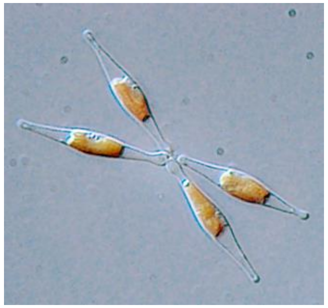
Titre du projet : Apport de la métabolomique dans l'identification des facteurs de transcription régulant l'accumulation de lipides par les microalgues au cours d'un stress

Auteurs: *Florence Mondeguer Laboratoire PHYCOTOXINES, Ifremer, Nantes*

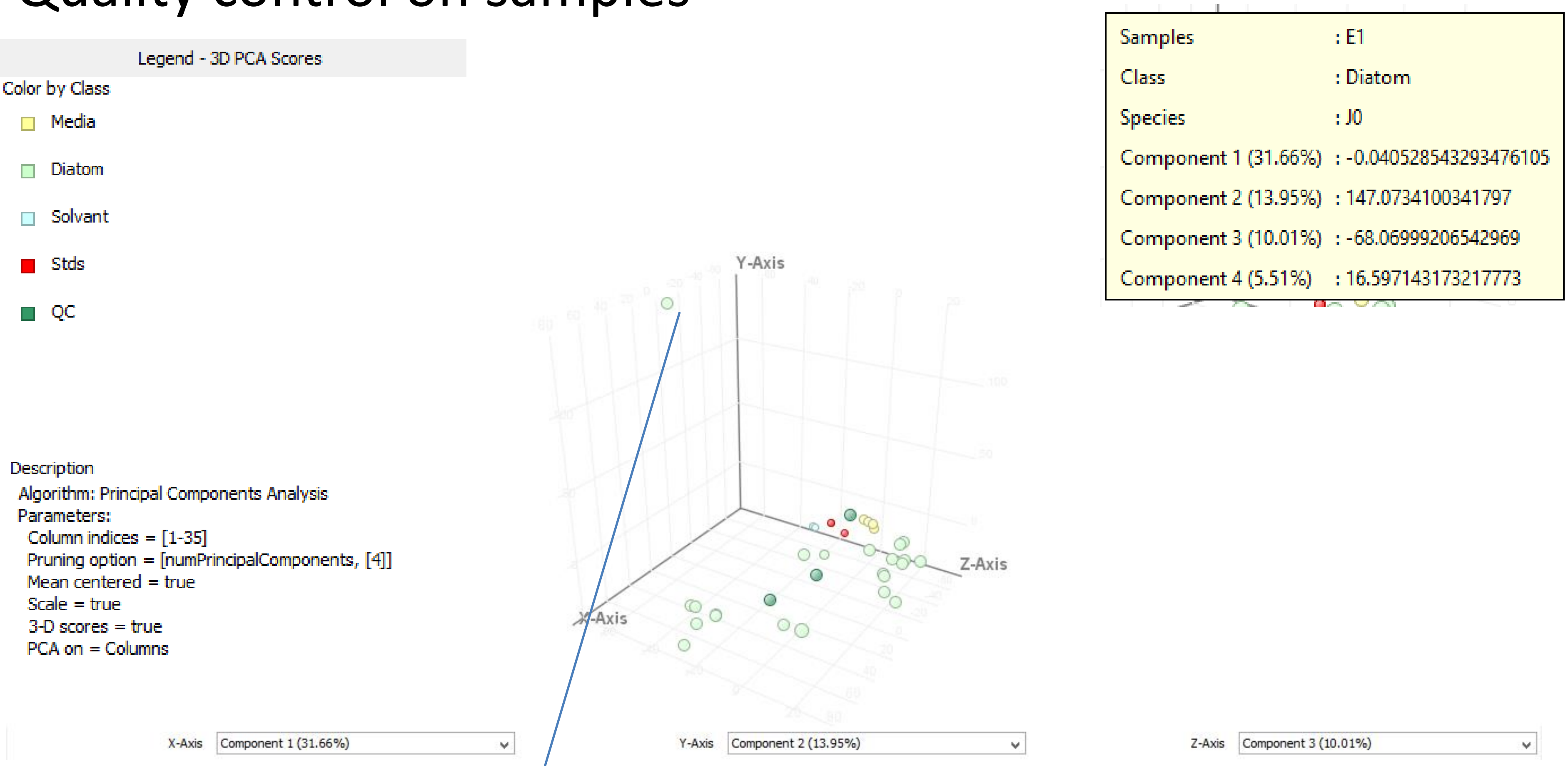


Résumé du projet :

Des expériences de culture (photobioréacteurs) de Phaeodactylum tricornutum, en condition de carence en azote, (favorisant la production de lipides ont été réalisés au laboratoire MMS. Le suivit physiologique et biochimique des cultures ainsi qu'une analyse transcriptomique (expression différentielle des gènes) permet de s'intéresser aux facteurs de transcription impliqués dans le contrôle de la voie de biosynthèse des lipides et des pigments chez cette diatomée. L'objectif du projet est de compléter cette étude **par une approche métabolomique qui permettra d'identifier de façon globale l'ensemble des métabolites différentiellement** formés permettant ainsi, associée à l'étude des gènes (transcriptomique), d'obtenir une vision intégrée de l'orientation des atomes de carbone dans les différentes voies de biosynthèse.

MassProfilerProfessional reprocessing

Quality control on samples



Legend - 3D PCA Scores

Color by Class

- 🟨 Media
- 🟩 Diatom
- 🟦 Solvant
- 🟥 Stds
- 🟩 QC

Description

Algorithm: Principal Components Analysis

Parameters:

Column indices = [1-35]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns

Samples : E1
Class : Diatom
Species : J0
Component 1 (31.66%) : -0.040528543293476105
Component 2 (13.95%) : 147.0734100341797
Component 3 (10.01%) : -68.06999206542969
Component 4 (5.51%) : 16.597143173217773

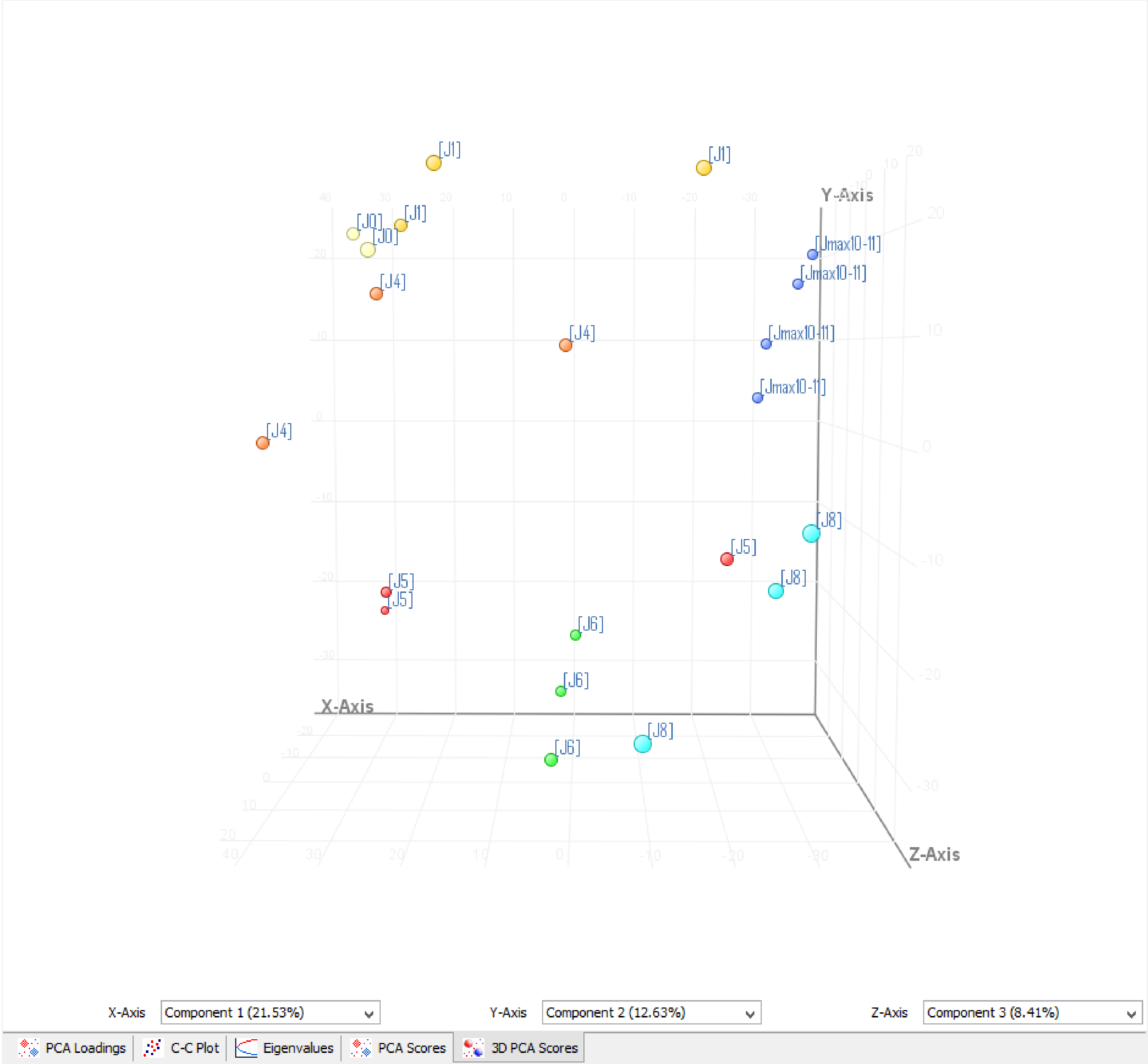
X-Axis Component 1 (31.66%)
Y-Axis Component 2 (13.95%)
Z-Axis Component 3 (10.01%)

Outlier ?

Ce premier échantilon a- t-il subit une pression particulière?

Ni non ce n’est pas très grave on peut le garder…

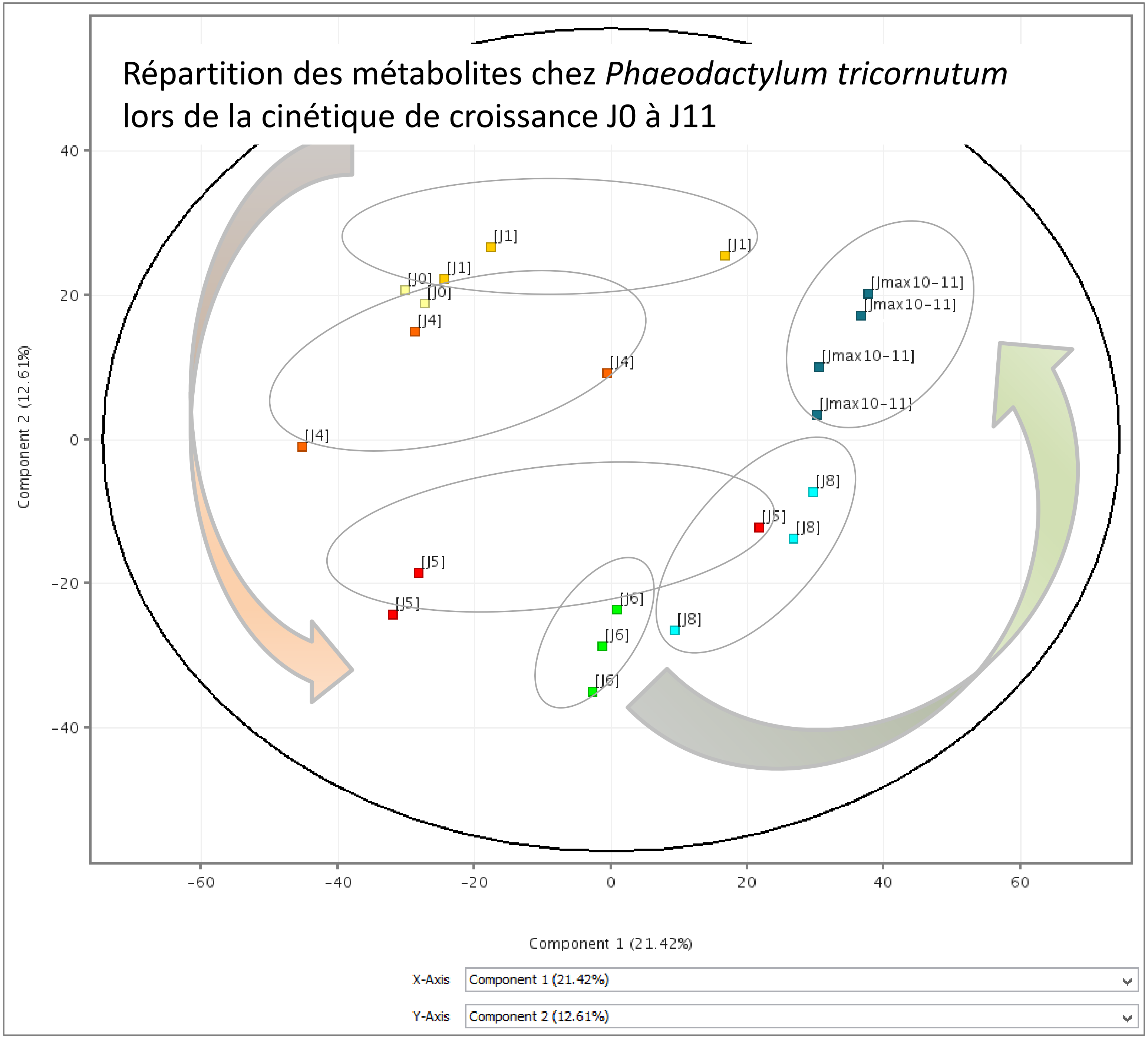
A décider



X-Axis Component 1 (21.53%)

Y-Axis Component 2 (12.63%)

Z-Axis Component 3 (8.41%)

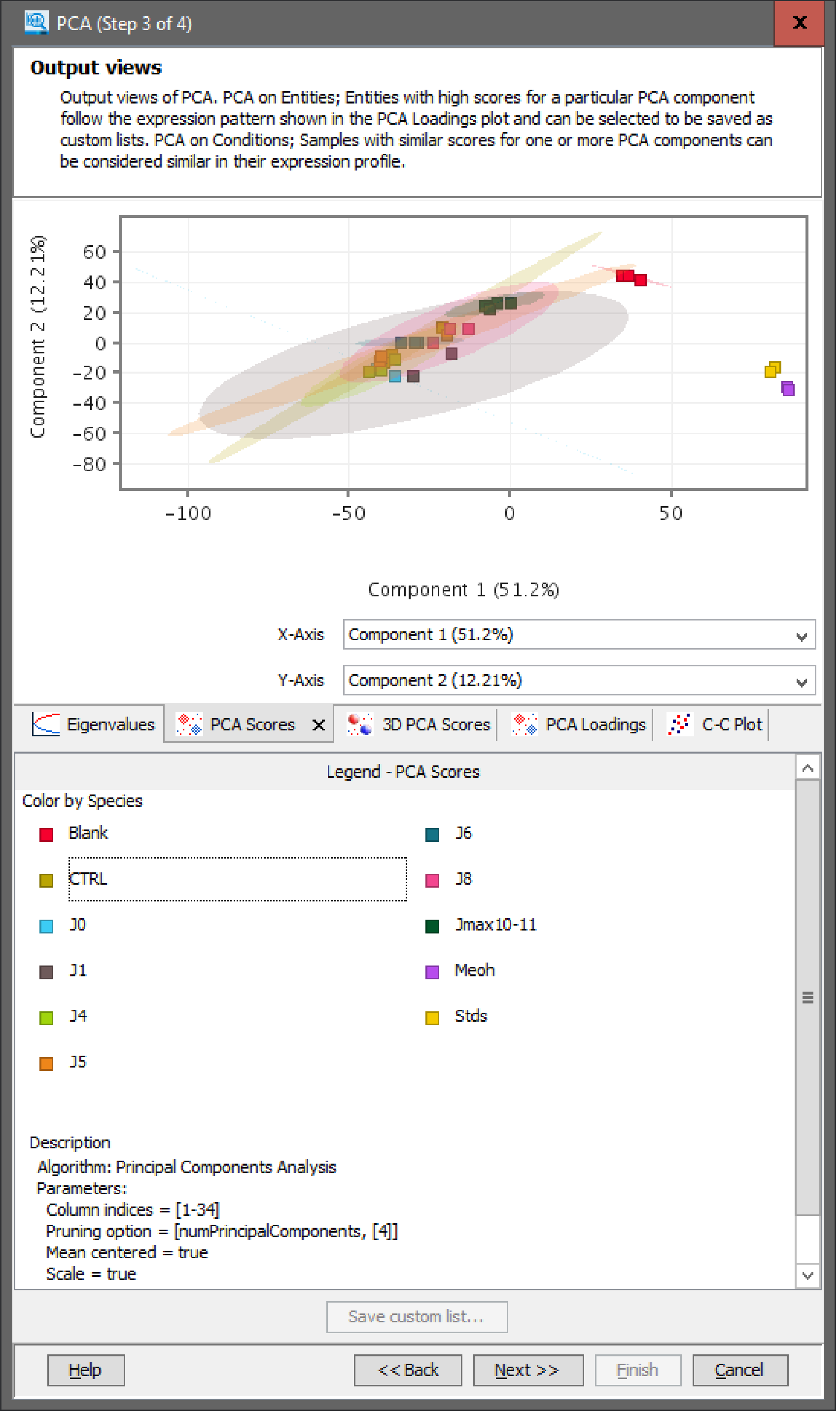


Répartition des métabolites chez *Phaeodactylum tricornutum* lors de la cinétique de croissance J0 à J11

X-Axis Component 1 (21.42%)

Y-Axis Component 2 (12.61%)

3D ACP ts samples



PCA (Step 3 of 4)

Output views

Output views of PCA. PCA on Entities; Entities with high scores for a particular PCA component follow the expression pattern shown in the PCA Loadings plot and can be selected to be saved as custom lists. PCA on Conditions; Samples with similar scores for one or more PCA components can be considered similar in their expression profile.

X-Axis Component 1 (51.2%)

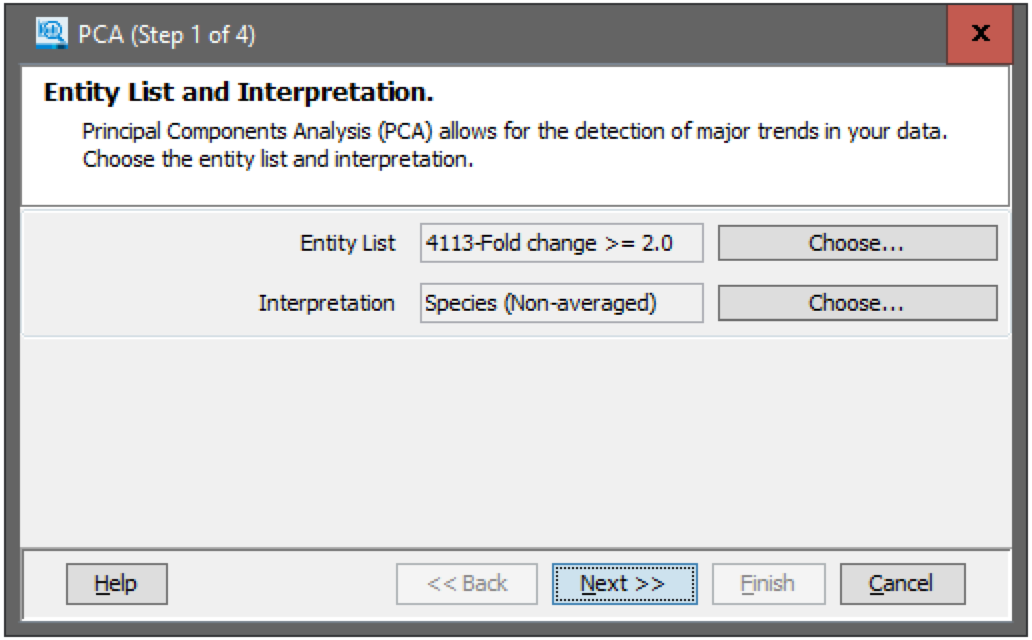
Y-Axis Component 2 (12.21%)

Legend - PCA Scores

Color by Species

🟥 Blank	🟦 J6
🟨 CTRL	🟥 J8
🟦 J0	🟩 Jmax10-11
🟫 J1	🟪 Meoh
🟩 J4	🟨 Stds
🟧 J5	

Description
Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-34]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true



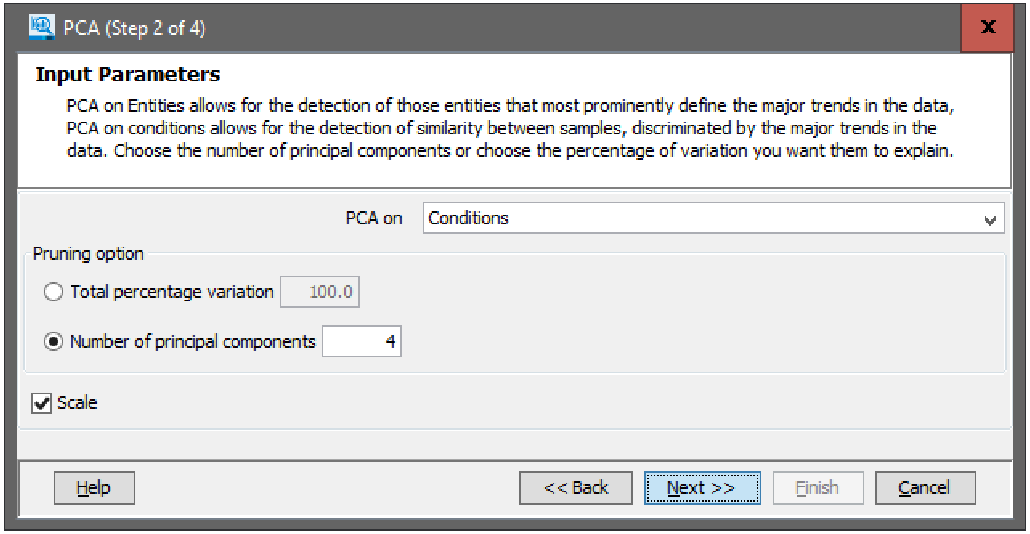
PCA (Step 1 of 4)

Entity List and Interpretation.

Principal Components Analysis (PCA) allows for the detection of major trends in your data. Choose the entity list and interpretation.

Entity List 4113-Fold change >= 2.0

Interpretation Species (Non-averaged)



PCA (Step 2 of 4)

Input Parameters

PCA on Entities allows for the detection of those entities that most prominently define the major trends in the data, PCA on conditions allows for the detection of similarity between samples, discriminated by the major trends in the data. Choose the number of principal components or choose the percentage of variation you want them to explain.

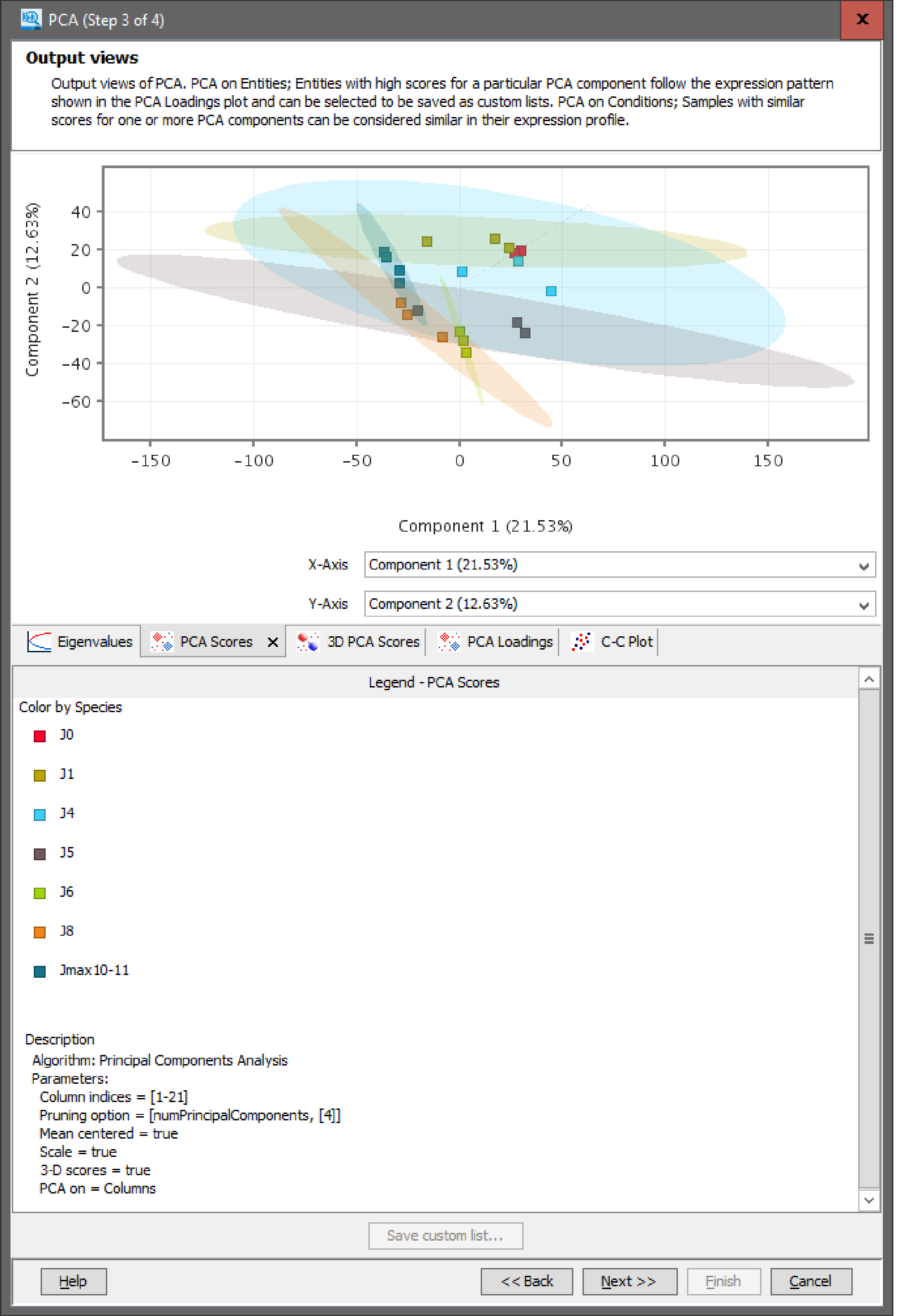
PCA on Conditions

Pruning option

○ Total percentage variation 100.0

● Number of principal components 4

☑ Scale



PCA (Step 3 of 4)

Output views

Output views of PCA. PCA on Entities; Entities with high scores for a particular PCA component follow the expression pattern shown in the PCA Loadings plot and can be selected to be saved as custom lists. PCA on Conditions; Samples with similar scores for one or more PCA components can be considered similar in their expression profile.

X-Axis Component 1 (21.53%)

Y-Axis Component 2 (12.63%)

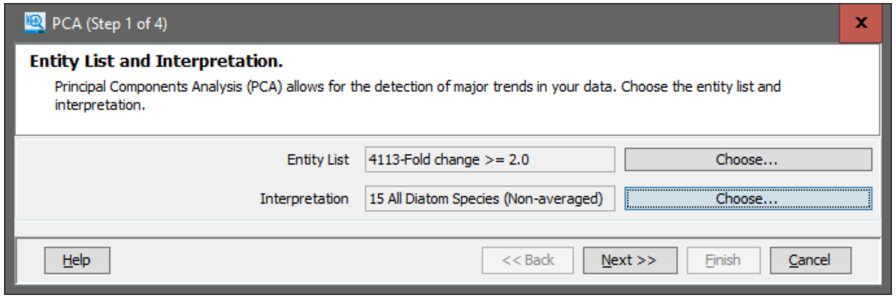
Legend - PCA Scores

Color by Species

- 🟥 J0
- 🟨 J1
- 🟦 J4
- ⬛ J5
- 🟩 J6
- 🟧 J8
- 🟦 Jmax10-11

Description

Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-21]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns



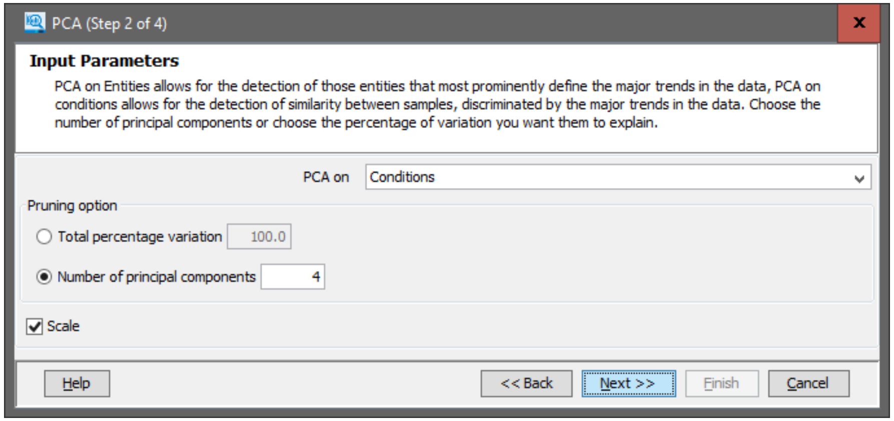
PCA (Step 1 of 4)

Entity List and Interpretation.

Principal Components Analysis (PCA) allows for the detection of major trends in your data. Choose the entity list and interpretation.

Entity List: 4113-Fold change >= 2.0

Interpretation: 15 All Diatom Species (Non-averaged)



PCA (Step 2 of 4)

Input Parameters

PCA on Entities allows for the detection of those entities that most prominently define the major trends in the data, PCA on conditions allows for the detection of similarity between samples, discriminated by the major trends in the data. Choose the number of principal components or choose the percentage of variation you want them to explain.

PCA on: Conditions

Pruning option

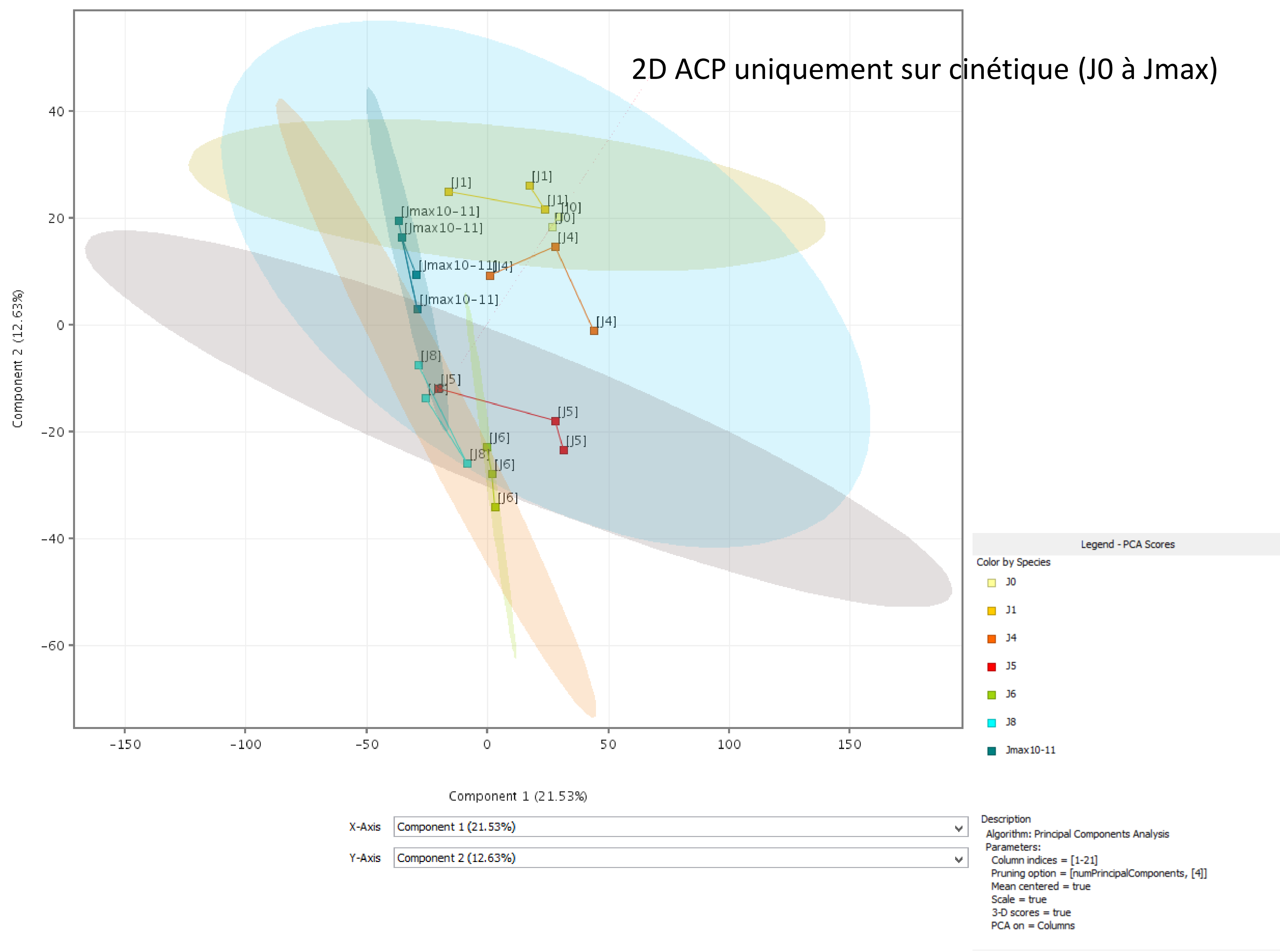
○ Total percentage variation 100.0

● Number of principal components 4

☑ Scale

3D ACP uniquement sur cinétique (J0 à Jmax)

2D ACP uniquement sur cinétique (J0 à Jmax)



X-Axis: Component 1 (21.53%)

Y-Axis: Component 2 (12.63%)

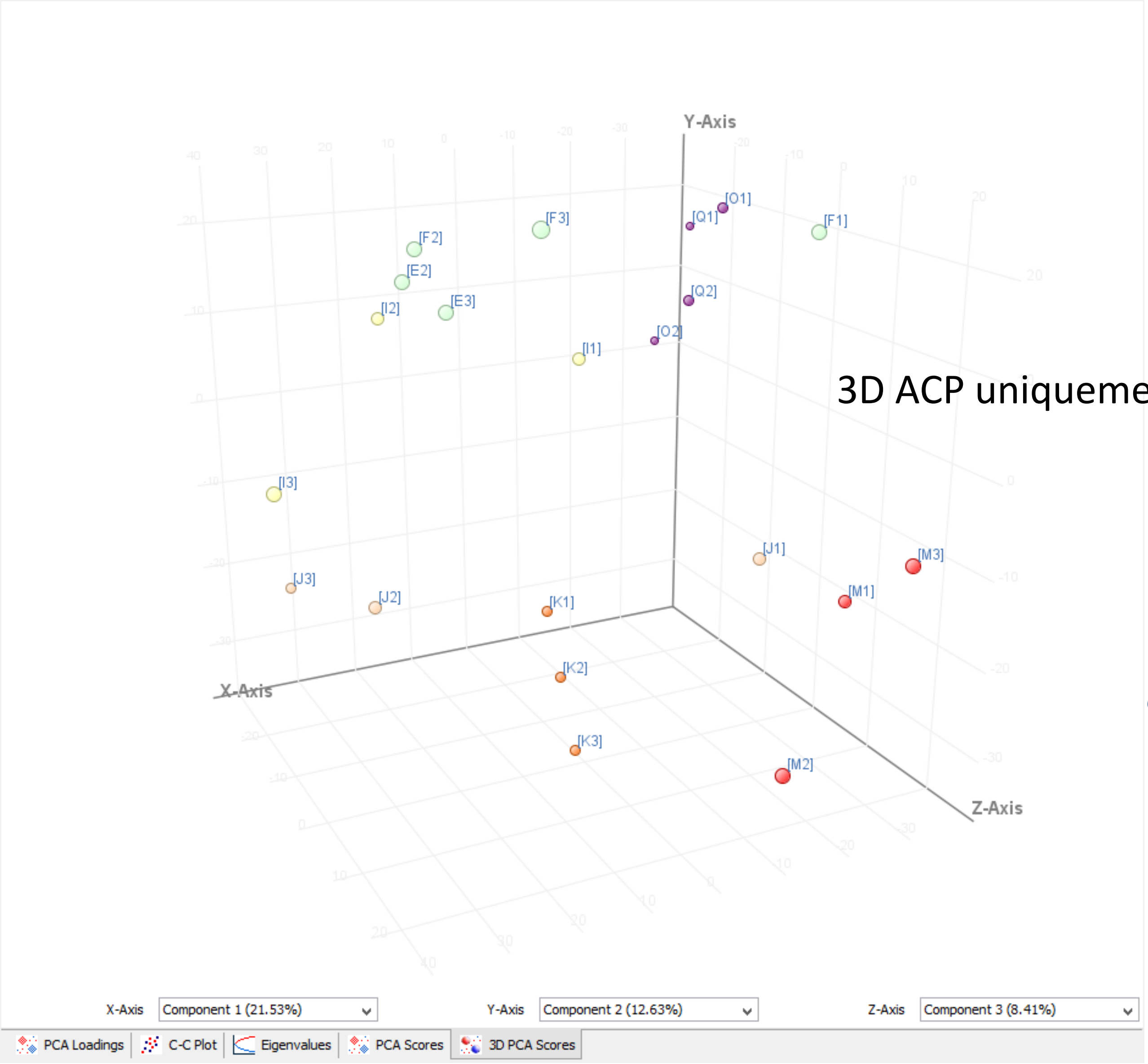
Description

Algorithm: Principal Components Analysis

Parameters:
- Column indices = [1-21]
- Pruning option = [numPrincipalComponents, [4]]
- Mean centered = true
- Scale = true
- 3-D scores = true
- PCA on = Columns

Comme demandé essai avec J0et J1 cumulés

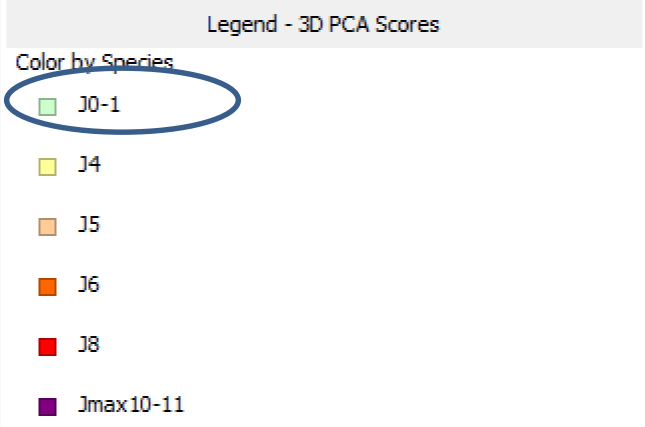
3D ACP uniquement sur cinétique (J0 à Jmax)



X-Axis Component 1 (21.53%)

Y-Axis Component 2 (12.63%)

Z-Axis Component 3 (8.41%)



Legend - 3D PCA Scores

Color by Species

- 🟩 J0-1
- 🟨 J4
- 🟧 J5
- 🟧 J6
- 🟥 J8
- 🟪 Jmax10-11

Description

Algorithm: Principal Components Analysis

Parameters:

Column indices = [1-21]

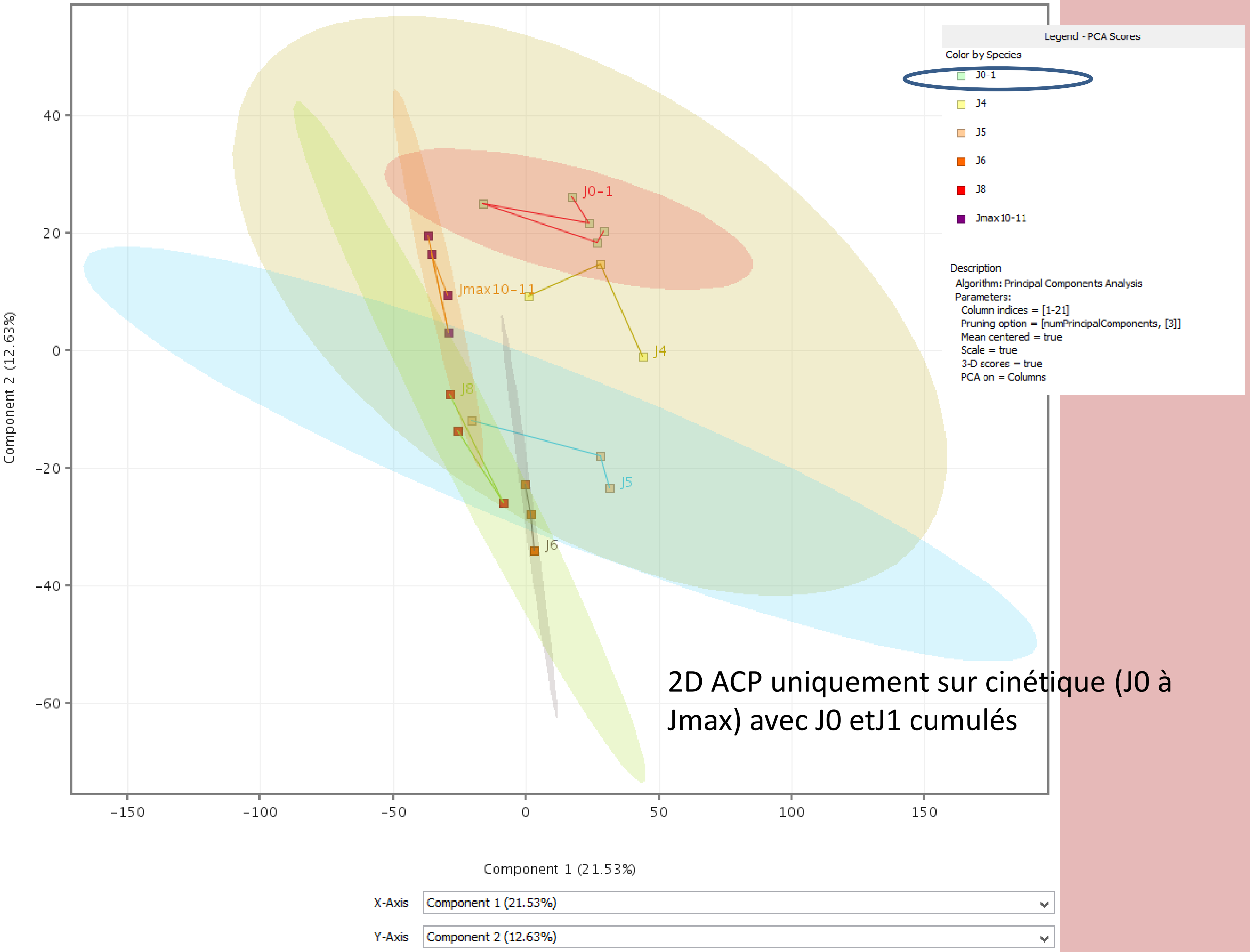
Pruning option = [numPrincipalComponents, [3]]

Mean centered = true

Scale = true

3-D scores = true

PCA on = Columns



Legend - PCA Scores

Color by Species

- 🟩 J0-1
- 🟨 J4
- 🟧 J5
- 🟧 J6
- 🟥 J8
- 🟪 Jmax10-11

Description

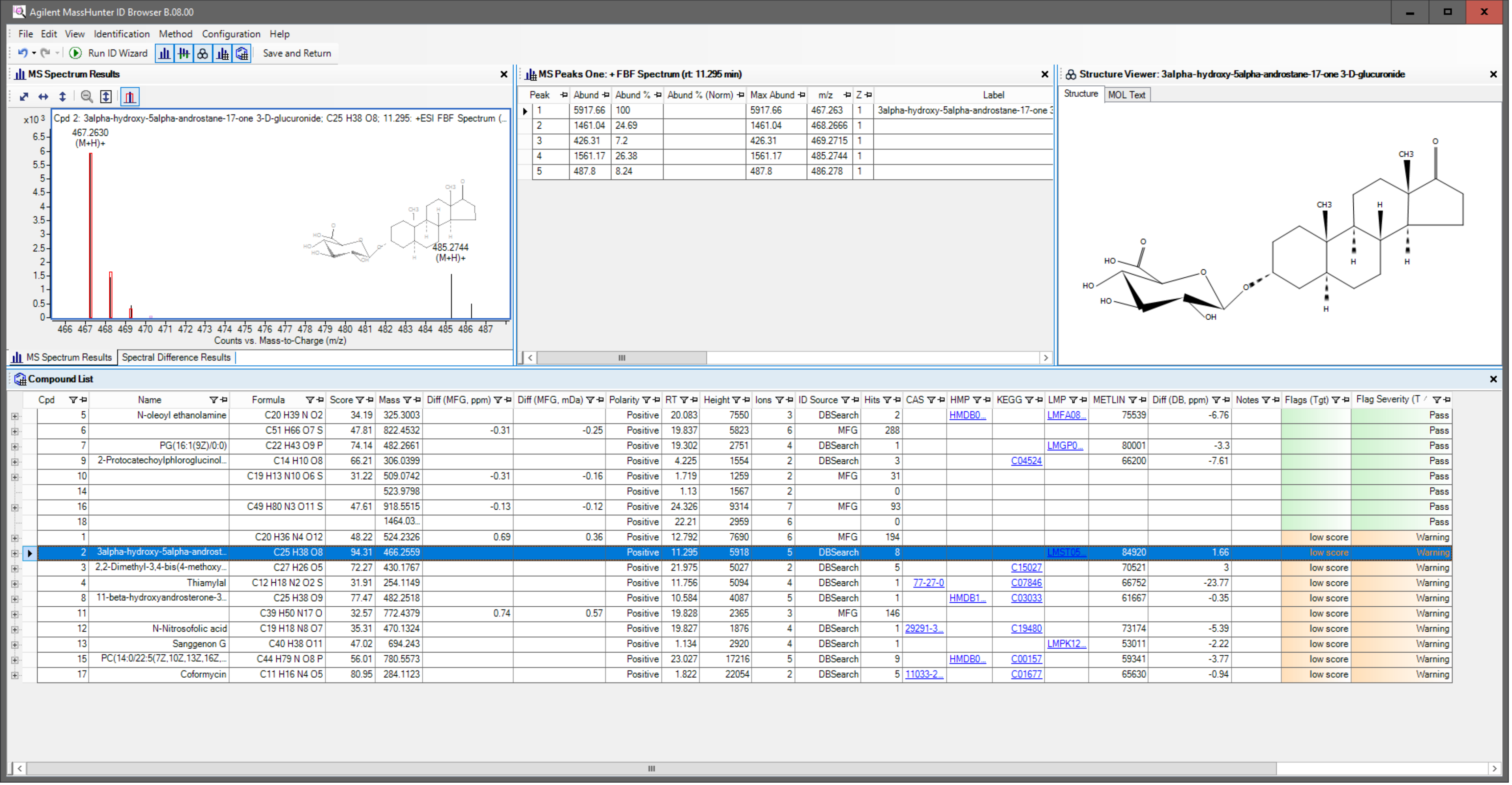
Algorithm: Principal Components Analysis

Parameters:

Column indices = [1-21]
Pruning option = [numPrincipalComponents, [3]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns

X-Axis Component 1 (21.53%)
Y-Axis Component 2 (12.63%)

2D ACP uniquement sur cinétique (J0 à Jmax) avec J0 etJ1 cumulés



Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label
1	5917.66	100		5917.66	467.263	1	3alpha-hydroxy-5alpha-androstane-17-one 3
2	1461.04	24.69		1461.04	468.2666	1	
3	426.31	7.2		426.31	469.2715	1	
4	1561.17	26.38		1561.17	485.2744	1	
5	487.8	8.24		487.8	486.278	1	

Cpd	Name	Formula	Score	Mass	Diff (MFG, ppm)	Diff (MFG, mDa)	Polarity	RT	Height	Ions	ID Source	Hits	CAS	HMP	KEGG	LMP	METLIN	Diff (DB, ppm)	Notes	Flags (Tgt)	Flag Severity (T
5	N-oleoyl ethanolamine	C20 H39 N O2	34.19	325.3003			Positive	20.083	7550	3	DBSearch	2		HMDB0...		LMFA08...	75539	-6.76			Pass
6		C51 H66 O7 S	47.81	822.4532	-0.31	-0.25	Positive	19.837	5823	6	MFG	288									Pass
7	PG(16:1(9Z)/0:0)	C22 H43 O9 P	74.14	482.2661			Positive	19.302	2751	4	DBSearch	1				LMGP0...	80001	-3.3			Pass
9	2-Protocatechoylphloroglucinol...	C14 H10 O8	66.21	306.0399			Positive	4.225	1554	2	DBSearch	3			C04524		66200	-7.61			Pass
10		C19 H13 N10 O6 S	31.22	509.0742	-0.31	-0.16	Positive	1.719	1259	2	MFG	31									Pass
14				523.9798			Positive	1.13	1567	2		0									Pass
16		C49 H80 N3 O11 S	47.61	918.5515	-0.13	-0.12	Positive	24.326	9314	7	MFG	93									Pass
18				1464.03...			Positive	22.21	2959	6		0									Pass
1		C20 H36 N4 O12	48.22	524.2326	0.69	0.36	Positive	12.792	7690	6	MFG	194								low score	Warning
2	3alpha-hydroxy-5alpha-androst...	C25 H38 O8	94.31	466.2559			Positive	11.295	5918	5	DBSearch	8				LMST05...	84920	1.66		low score	Warning
3	2,2-Dimethyl-3,4-bis(4-methoxy...	C27 H26 O5	72.27	430.1767			Positive	21.975	5027	2	DBSearch	5			C15027		70521	3		low score	Warning
4	Thiamylal	C12 H18 N2 O2 S	31.91	254.1149			Positive	11.756	5094	4	DBSearch	1	77-27-0		C07846		66752	-23.77		low score	Warning
8	11-beta-hydroxyandrosterone-3...	C25 H38 O9	77.47	482.2518			Positive	10.584	4087	5	DBSearch	1		HMDB1...	C03033		61667	-0.35		low score	Warning
11		C39 H50 N17 O	32.57	772.4379	0.74	0.57	Positive	19.828	2365	3	MFG	146								low score	Warning
12	N-Nitrosofolic acid	C19 H18 N8 O7	35.31	470.1324			Positive	19.827	1876	4	DBSearch	1	29291-3...		C19480		73174	-5.39		low score	Warning
13	Sanggenon G	C40 H38 O11	47.02	694.243			Positive	1.134	2920	4	DBSearch	1				LMPK12...	53011	-2.22		low score	Warning
15	PC(14:0/22:5(7Z,10Z,13Z,16Z,...	C44 H79 N O8 P	56.01	780.5573			Positive	23.027	17216	5	DBSearch	9		HMDB0...	C00157		59341	-3.77		low score	Warning
17	Coformycin	C11 H16 N4 O5	80.95	284.1123			Positive	1.822	22054	2	DBSearch	5	11033-2...		C01677		65630	-0.94		low score	Warning

Secondary metabolite identification for 18 Entities unic J0:

Best Know: 3/18

- Cpd 7: PG(16:1(9Z)/0:0); C22H43O9P@19.302 Score: 74.14

PG(16:1(9Z)/0:0) is a lysophosphatidylglycerol 16:1.

lyso-PG (16:1) :Changes of lipid molecular species during cold stress

…..next slide

Secondary metabolite identification for 18 Entities unic J0:

Best Know: 3/18

- Cpd 7: PG(16:1(9Z)/0:0); $C_{22}H_{43}O_9P$@19.302 Score: 74.14

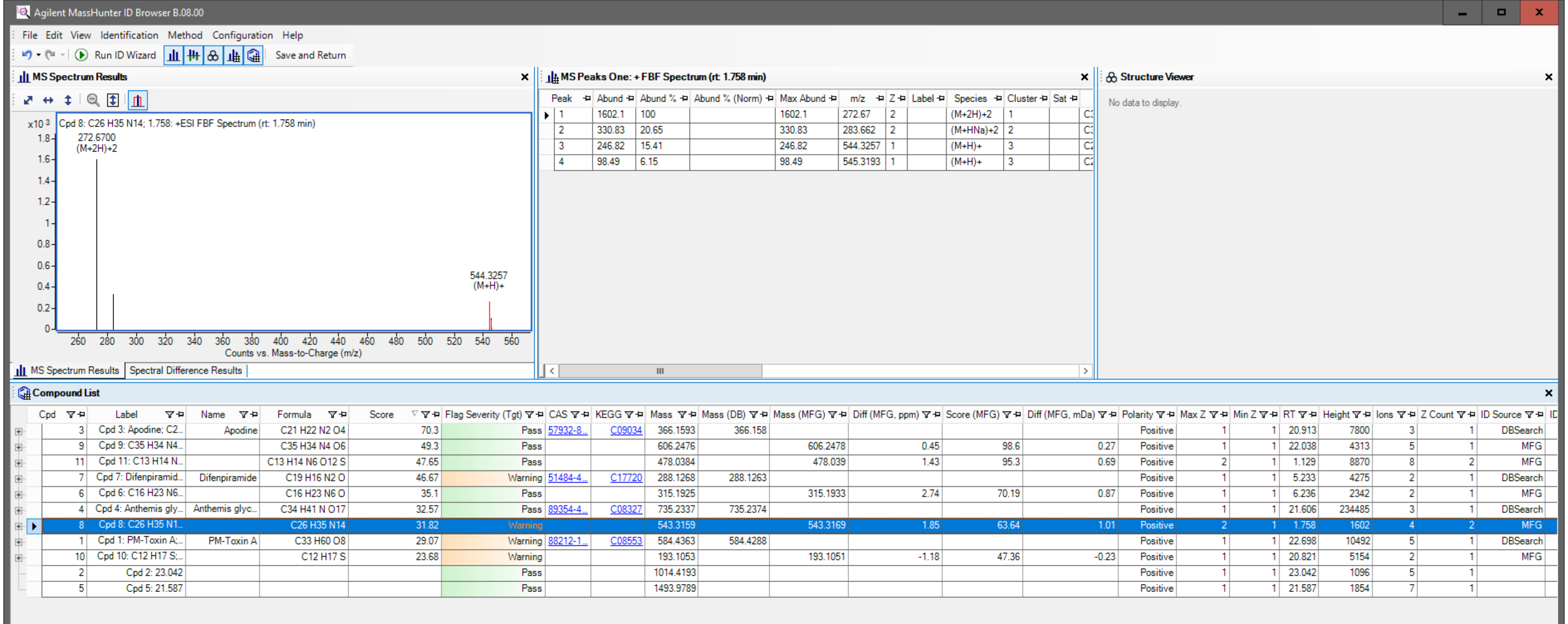
PG(16:1(9Z)/0:0) is a lysophosphatidylglycerol 16:1.
lyso-PG (16:1) :Changes of lipid molecular species during cold stress

- Cpd 9: 2-Protocatechoylphloroglucinolcarboxylate; $C_{14}H_{10}O_8$@4.225 score: 66.21

2-Protocatechoylphloroglucinolcarboxylate= **2-(3,4-Dihydroxybenzoyloxy)-4,6-dihydroxybenzoate**: A metabolite of quercetin, an abundant flavonoid found in edible vegetables, grains and fruits which is used as an ingredient in supplements, beverages, or foods. It is a dihydroxybenzoic acid and a benzoate ester. It is a conjugate acid of a 2-(3,4-dihydroxybenzoyloxy)-4,6-dihydroxybenzoate.

- Cpd 5: N-oleoyl ethanolamine; $C_{20}H_{39}NO_2$@20.083 score:34.19

Oleoylethanolamide (OEA or NOE) is an N-acylethanolamine.
N-Acylethanolamines (NAEs) constitute a class of lipid compounds naturally present in both animal and plant membranes as constituents of the membrane-bound phospholipid,



MS Peaks One: + FBF Spectrum (rt: 1.758 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Species	Cluster	Sat
1	1602.1	100		1602.1	272.67	2		(M+2H)+2	1	
2	330.83	20.65		330.83	283.662	2		(M+HNa)+2	2	
3	246.82	15.41		246.82	544.3257	1		(M+H)+	3	
4	98.49	6.15		98.49	545.3193	1		(M+H)+	3	

Compound List

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT	Height	Ions	Z Count	ID Source
3	Cpd 3: Apodine; C2...	Apodine	C21 H22 N2 O4	70.3	Pass	57932-8...	C09034	366.1593	366.158					Positive	1	1	20.913	7800	3	1	DBSearch
9	Cpd 9: C35 H34 N4...		C35 H34 N4 O6	49.3	Pass			606.2476		606.2478	0.45	98.6	0.27	Positive	1	1	22.038	4313	5	1	MFG
11	Cpd 11: C13 H14 N...		C13 H14 N6 O12 S	47.65	Pass			478.0384		478.039	1.43	95.3	0.69	Positive	2	1	1.129	8870	8	2	MFG
7	Cpd 7: Difenpiramid...	Difenpiramide	C19 H16 N2 O	46.67	Warning	51484-4...	C17720	288.1268	288.1263					Positive	1	1	5.233	4275	2	1	DBSearch
6	Cpd 6: C16 H23 N6...		C16 H23 N6 O	35.1	Pass			315.1925		315.1933	2.74	70.19	0.87	Positive	1	1	6.236	2342	2	1	MFG
4	Cpd 4: Anthemis gly...	Anthemis glyc...	C34 H41 N O17	32.57	Pass	89354-4...	C08327	735.2337	735.2374					Positive	1	1	21.606	234485	3	1	DBSearch
8	Cpd 8: C26 H35 N1...		C26 H35 N14	31.82	Warning			543.3159		543.3169	1.85	63.64	1.01	Positive	2	1	1.758	1602	4	2	MFG
1	Cpd 1: PM-Toxin A;...	PM-Toxin A	C33 H60 O8	29.07	Warning	88212-1...	C08553	584.4363	584.4288					Positive	1	1	22.698	10492	5	1	DBSearch
10	Cpd 10: C12 H17 S;...		C12 H17 S	23.68	Warning			193.1053		193.1051	-1.18	47.36	-0.23	Positive	1	1	20.821	5154	2	1	MFG
2	Cpd 2: 23.042				Pass			1014.4193						Positive	1	1	23.042	1096	5	1	
5	Cpd 5: 21.587				Pass			1493.9789						Positive	1	1	21.587	1854	7	1	

Secondary metabolite identification for 11 Entities unic J1:

Best Know: 1/11 (mais 2 choix)

Cpd 3: Octocrylene; C24H27NO2@20.913,Octocrylene Score:78.28

Octocrylene is an organic compound used as an ingredient in sunscreens and cosmetics?

Autre possibilité avec un score légèrement plus petit si aucune contamination n’est envisageable alors:

Cpd 3: Apodine;C21H22N2O4 @20.913 Score:70.3

Phytochemical compounds Alkaloids

Some of the allelopathic compounds from algae and seaweeds have been isolated and characterized including alkaloids and marine diatom *Phaeodactylum tricornutum* is known to exude allelochemicals with negative effects.

Secondary metabolite identification for 9 Entities unic J4 :

Best Know: 3/9

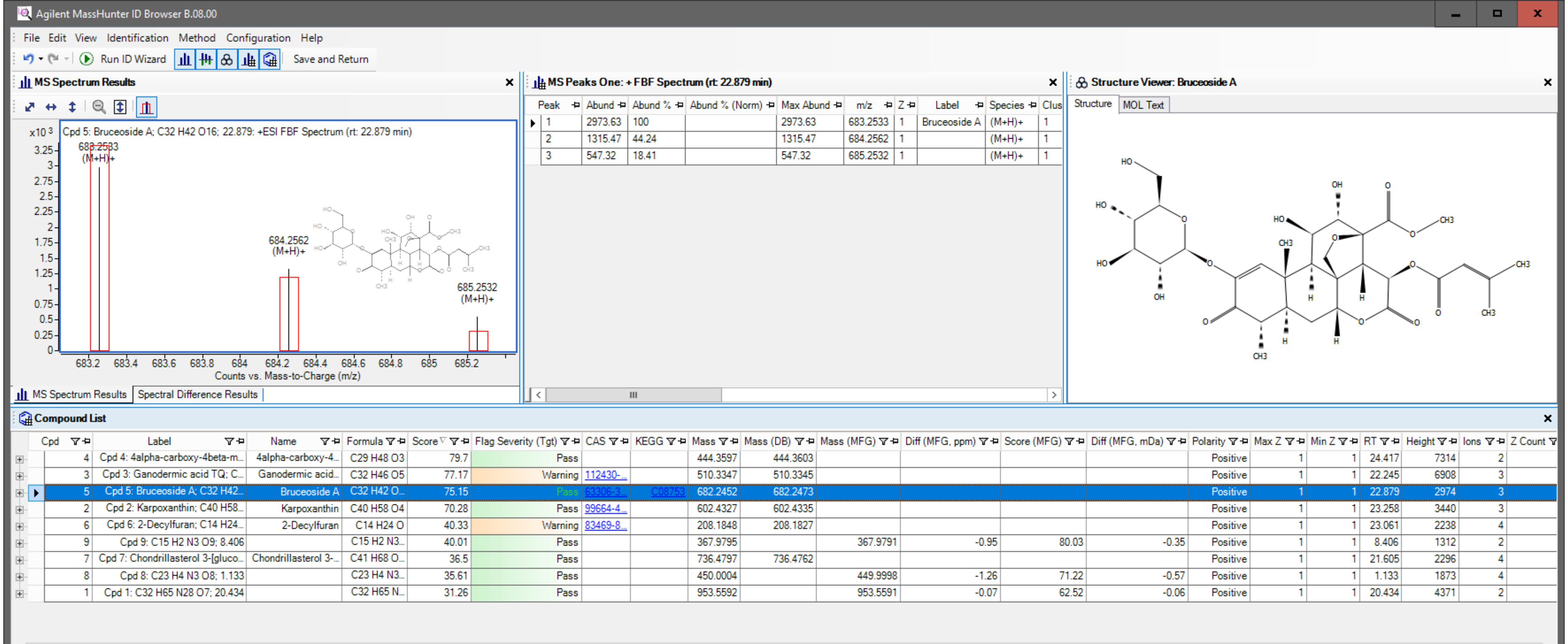
- Cpd 4: 4alpha-carboxy-4beta-methyl-5alpha-cholesta-8-en-3beta-ol OR 3β-hydroxysteroid-4α-carboxylate; $C_{29}H_{48}O_3$ @24.417 Score:79.7

cholesterol biosynthesis II (via 24,25-dihydrolanosterol).

Superclasses: a steroid → a hydroxysteroid → a sterol → a 3beta-hydroxysteroid

Steroids are abundant in the environment. Large amounts of steroids and their derivatives are synthesized by eukaryotes, and these molecules play very important and diverse roles and include hormones, detergents that facilitate the absorption of lipids by the intestine, and membrane constituents. Some of them, cholesterol and related compounds, are ubiquitous as membrane constituent of eukaryotes (for instance, up to 10% of the dry mass of yeast is ergosterol) and as the precursors of all steroid hormones, vitamin D, and the bile acids.

Interestingly, with exception of methane-oxidizing bacteria that contain relatively large amounts of sterols, sterols are absent from most prokaryotes. However, many bacterial membranes contain hopanoids, which are similar pentacyclic sterol-like molecules [Chiang08].



MS Peaks One: + FBF Spectrum (rt: 22.879 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Species	Clus
1	2973.63	100		2973.63	683.2533	1	Bruceoside A	(M+H)+	1
2	1315.47	44.24		1315.47	684.2562	1		(M+H)+	1
3	547.32	18.41		547.32	685.2532	1		(M+H)+	1

Compound List

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT	Height	Ions	Z Count
4	Cpd 4: 4alpha-carboxy-4beta-m...	4alpha-carboxy-4...	C29 H48 O3	79.7	Pass			444.3597	444.3603					Positive	1	1	24.417	7314	2	
3	Cpd 3: Ganodermic acid TQ; C...	Ganodermic acid...	C32 H46 O5	77.17	Warning	112430-...		510.3347	510.3345					Positive	1	1	22.245	6908	3	
5	Cpd 5: Bruceoside A; C32 H42...	Bruceoside A	C32 H42 O...	75.15	Pass	63306-3...	C08753	682.2452	682.2473					Positive	1	1	22.879	2974	3	
2	Cpd 2: Karpoxanthin; C40 H58...	Karpoxanthin	C40 H58 O4	70.28	Pass	99664-4...		602.4327	602.4335					Positive	1	1	23.258	3440	3	
6	Cpd 6: 2-Decylfuran; C14 H24...	2-Decylfuran	C14 H24 O	40.33	Warning	83469-8...		208.1848	208.1827					Positive	1	1	23.061	2238	4	
9	Cpd 9: C15 H2 N3 O9; 8.406		C15 H2 N3...	40.01	Pass			367.9795		367.9791	-0.95	80.03	-0.35	Positive	1	1	8.406	1312	2	
7	Cpd 7: Chondrillasterol 3-[gluco...	Chondrillasterol 3-...	C41 H68 O...	36.5	Pass			736.4797	736.4762					Positive	1	1	21.605	2296	4	
8	Cpd 8: C23 H4 N3 O8; 1.133		C23 H4 N3...	35.61	Pass			450.0004		449.9998	-1.26	71.22	-0.57	Positive	1	1	1.133	1873	4	
1	Cpd 1: C32 H65 N28 O7; 20.434		C32 H65 N...	31.26	Pass			953.5592		953.5591	-0.07	62.52	-0.06	Positive	1	1	20.434	4371	2	

Secondary metabolite identification for 9 Entities unic J4 :

Best Know: 3/9

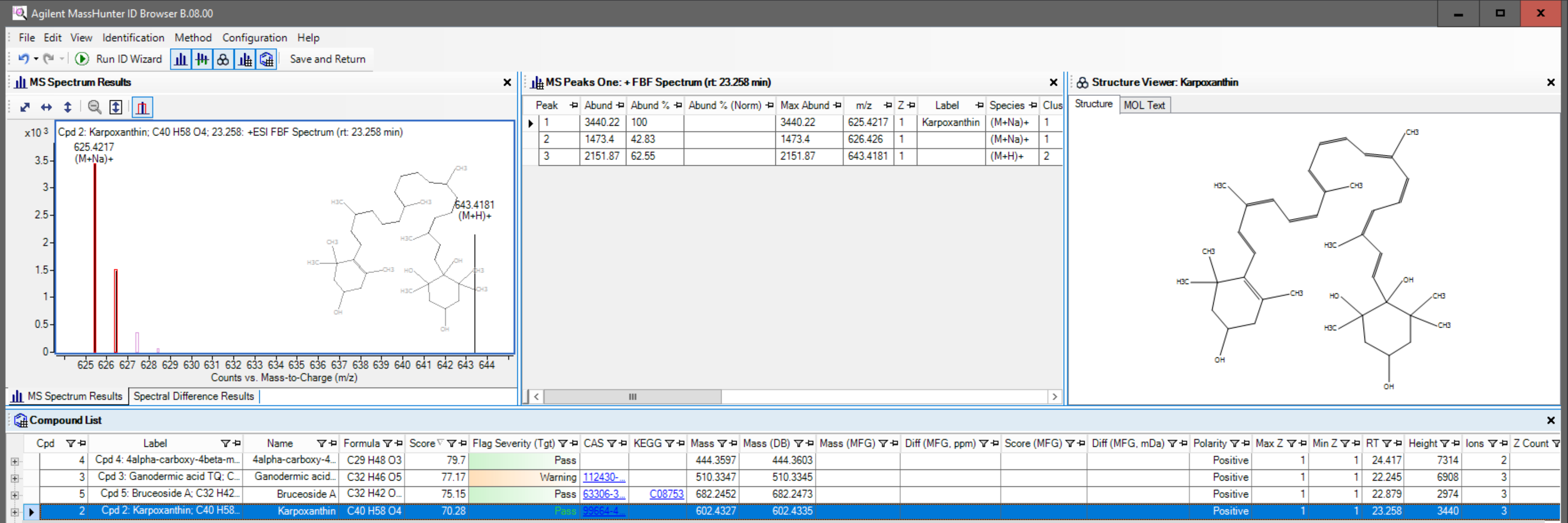
- Cpd 5: Bruceoside A; $C_{32}H_{42}O_{16}$ @ 22.879 Sore:75.15

Superclasses: a lipid → an isoprenoid → a terpenoid → a triterpenoid

Bruceoside A is a triterpenoid saponin

Plant triterpenoids constitute a diverse class of organic compounds that play a major role in development, plant defence and environmental interaction. Several triterpenes have demonstrated potential as pharmaceuticals.

For example, some have reported the production of the triterpenes betulin and its precursor lupeol in the photosynthetic diatom *Phaeodactylum tricornutum*



Cpd 2: Karpoxanthin; C40 H58 O4; 23.258: +ESI FBF Spectrum (rt: 23.258 min)

MS Peaks One: + FBF Spectrum (rt: 23.258 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Species	Clus
1	3440.22	100		3440.22	625.4217	1	Karpoxanthin	(M+Na)+	1
2	1473.4	42.83		1473.4	626.426	1		(M+Na)+	1
3	2151.87	62.55		2151.87	643.4181	1		(M+H)+	2

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT	Height	Ions	Z Count
4	Cpd 4: 4alpha-carboxy-4beta-m...	4alpha-carboxy-4...	C29 H48 O3	79.7	Pass			444.3597	444.3603					Positive	1	1	24.417	7314	2	
3	Cpd 3: Ganodermic acid TQ; C...	Ganodermic acid...	C32 H46 O5	77.17	Warning	112430-...		510.3347	510.3345					Positive	1	1	22.245	6908	3	
5	Cpd 5: Bruceoside A; C32 H42...	Bruceoside A	C32 H42 O...	75.15	Pass	63306-3...	C08753	682.2452	682.2473					Positive	1	1	22.879	2974	3	
2	Cpd 2: Karpoxanthin; C40 H58...	Karpoxanthin	C40 H58 O4	70.28	Pass	99664-4...		602.4327	602.4335					Positive	1	1	23.258	3440	3	

Secondary metabolite identification for 9 Entities unic J4 :

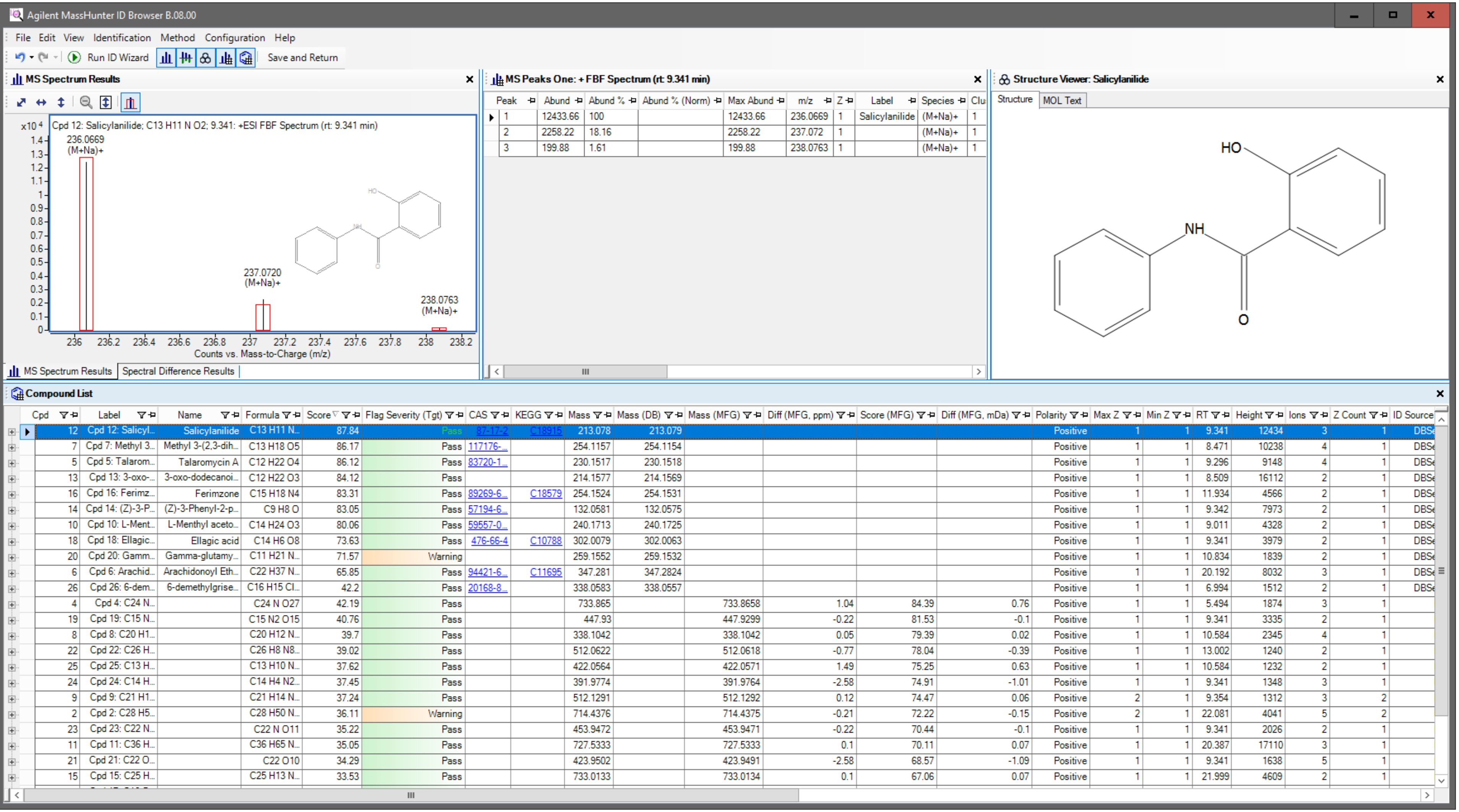
Best Know: 3/9

- Cpd 2: Karpoxanthin; $C_{40}H_{58}O_4$@23.258 Score 70.28

Furthermore, annually, more than 20 new structures of carotenoids are reported ...

from diatom Phaeodactylum tricornutum (Photosynthetic pigments in diatoms. P Kuczynska, M Jemiola-Rzeminska, K Strzalka - Marine drugs, 2015 - mdpi.com)

Carotenoids are C40 isoprenoids which consist of eight isoprene units and can be divided in two major groups: carotenes and xanthophylls. Carotenes are linear or cyclized hydrocarbons such as lycopene, α-carotene and β-carotene. Xanthophylls are oxygenated derivatives (epoxy, keto or hydroxyl groups) of carotenes; for example: lutein and zeaxanthin. The carotenoid composition varies from species to species; the concentration and composition of xanthophylls are affected by light intensity and the accumulation of specific carotenoids in fruit and flower chromoplasts is a highly, developmentally regulated process [Fraser94, Giuliano93]. Important carotenoids variations are observed during fruit ripening (for review, see [Ronen99]). Higher plant chloroplasts typically accumulate lutein, β-carotene, violaxanthin and neoxanthin in the thylakoid membrane-bound photosystems [Peter91, Ryberg93]. β-Carotene is generally found in the reaction center where it plays a critical photoprotective role by quenching triplet chlorophyll and singlet oxygen, and can undergo rapid degradation during photooxidation [Young93a]. Adjacent to the reaction centers, in the core complex proteins, β-carotene and lutein can be found [Peter91, Bassi93]. Finally, the surrounding antenna complexes contain xanthophylls (lutein, violaxanthin and neoxanthin) [Peter91, Bassi93]. In the chromoplasts of ripening fruits and flower petals, and in the chloroplasts of senescing leaves, the carotenoids are found in membranes or in oil bodies or other structures within the stroma.



Cpd 12: Salicylanilide; C13 H11 N O2; 9.341: +ESI FBF Spectrum (rt: 9.341 min)

MS Peaks One: + FBF Spectrum (rt: 9.341 min)

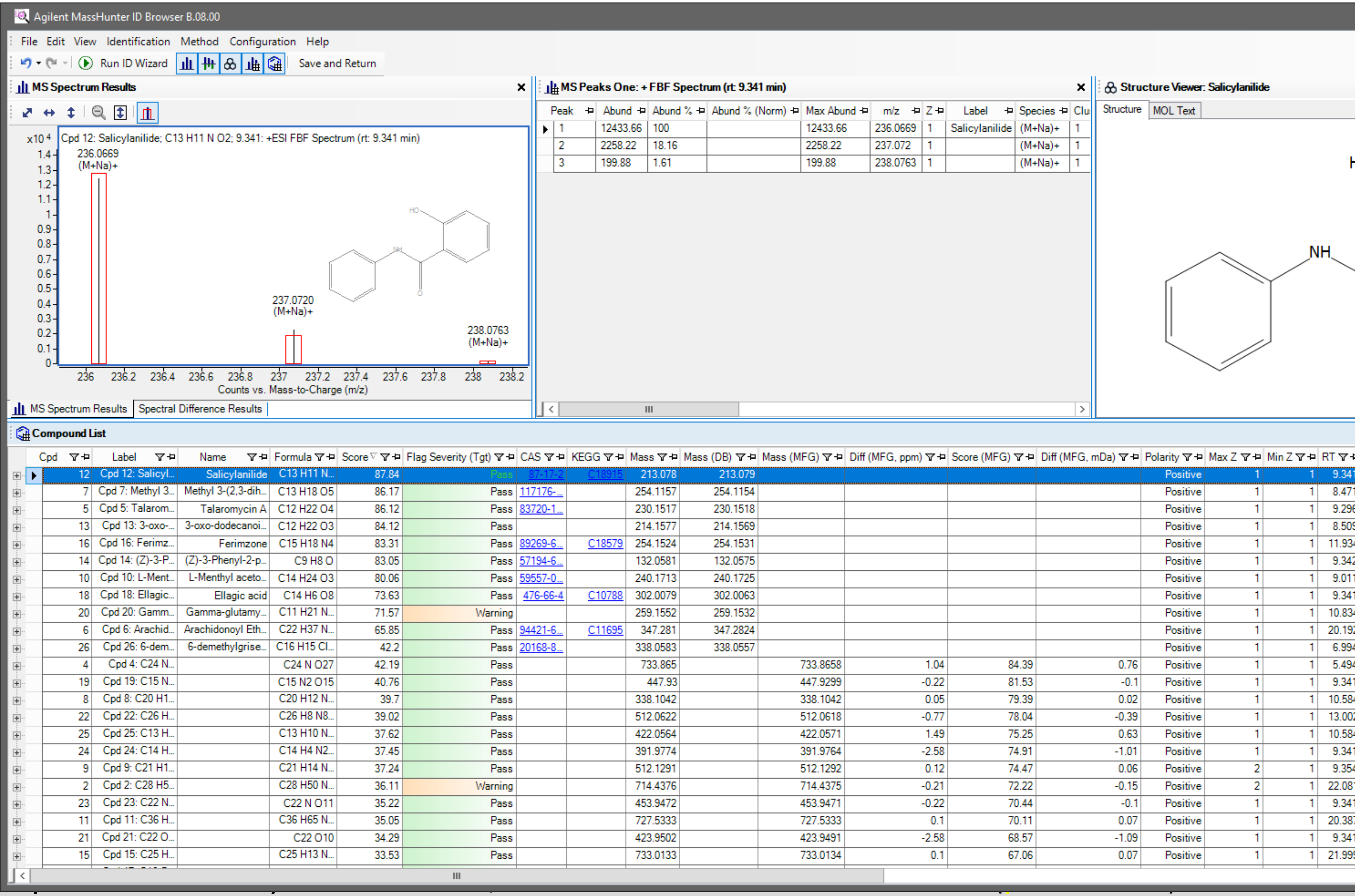
Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Species	Clu
1	12433.66	100		12433.66	236.0669	1	Salicylanilide	(M+Na)+	1
2	2258.22	18.16		2258.22	237.072	1		(M+Na)+	1
3	199.88	1.61		199.88	238.0763	1		(M+Na)+	1

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT	Height	Ions	Z Count	ID Source
12	Cpd 12: Salicyl...	Salicylanilide	C13 H11 N...	87.84	Pass	87-17-2	C18915	213.078	213.079					Positive	1	1	9.341	12434	3	1	DBSe
7	Cpd 7: Methyl 3...	Methyl 3-(2,3-dih...	C13 H18 O5	86.17	Pass	117176-...		254.1157	254.1154					Positive	1	1	8.471	10238	4	1	DBSe
5	Cpd 5: Talarom...	Talaromycin A	C12 H22 O4	86.12	Pass	83720-1...		230.1517	230.1518					Positive	1	1	9.296	9148	4	1	DBSe
13	Cpd 13: 3-oxo-...	3-oxo-dodecanoi...	C12 H22 O3	84.12	Pass			214.1577	214.1569					Positive	1	1	8.509	16112	2	1	DBSe
16	Cpd 16: Ferimz...	Ferimzone	C15 H18 N4	83.31	Pass	89269-6...	C18579	254.1524	254.1531					Positive	1	1	11.934	4566	2	1	DBSe
14	Cpd 14: (Z)-3-P...	(Z)-3-Phenyl-2-p...	C9 H8 O	83.05	Pass	57194-6...		132.0581	132.0575					Positive	1	1	9.342	7973	2	1	DBSe
10	Cpd 10: L-Ment...	L-Menthyl aceto...	C14 H24 O3	80.06	Pass	59557-0...		240.1713	240.1725					Positive	1	1	9.011	4328	2	1	DBSe
18	Cpd 18: Ellagic...	Ellagic acid	C14 H6 O8	73.63	Pass	476-66-4	C10788	302.0079	302.0063					Positive	1	1	9.341	3979	2	1	DBSe
20	Cpd 20: Gamm...	Gamma-glutamy...	C11 H21 N...	71.57	Warning			259.1552	259.1532					Positive	1	1	10.834	1839	2	1	DBSe
6	Cpd 6: Arachid...	Arachidonoyl Eth...	C22 H37 N...	65.85	Pass	94421-6...	C11695	347.281	347.2824					Positive	1	1	20.192	8032	3	1	DBSe
26	Cpd 26: 6-dem...	6-demethylgrise...	C16 H15 Cl...	42.2	Pass	20168-8...		338.0583	338.0557					Positive	1	1	6.994	1512	2	1	DBSe
4	Cpd 4: C24 N...		C24 N O27	42.19	Pass			733.865		733.8658	1.04	84.39	0.76	Positive	1	1	5.494	1874	3	1	
19	Cpd 19: C15 N...		C15 N2 O15	40.76	Pass			447.93		447.9299	-0.22	81.53	-0.1	Positive	1	1	9.341	3335	2	1	
8	Cpd 8: C20 H1...		C20 H12 N...	39.7	Pass			338.1042		338.1042	0.05	79.39	0.02	Positive	1	1	10.584	2345	4	1	
22	Cpd 22: C26 H...		C26 H8 N8...	39.02	Pass			512.0622		512.0618	-0.77	78.04	-0.39	Positive	1	1	13.002	1240	2	1	
25	Cpd 25: C13 H...		C13 H10 N...	37.62	Pass			422.0564		422.0571	1.49	75.25	0.63	Positive	1	1	10.584	1232	2	1	
24	Cpd 24: C14 H...		C14 H4 N2...	37.45	Pass			391.9774		391.9764	-2.58	74.91	-1.01	Positive	1	1	9.341	1348	3	1	
9	Cpd 9: C21 H1...		C21 H14 N...	37.24	Pass			512.1291		512.1292	0.12	74.47	0.06	Positive	2	1	9.354	1312	3	2	
2	Cpd 2: C28 H5...		C28 H50 N...	36.11	Warning			714.4376		714.4375	-0.21	72.22	-0.15	Positive	2	1	22.081	4041	5	2	
23	Cpd 23: C22 N...		C22 N O11	35.22	Pass			453.9472		453.9471	-0.22	70.44	-0.1	Positive	1	1	9.341	2026	2	1	
11	Cpd 11: C36 H...		C36 H65 N...	35.05	Pass			727.5333		727.5333	0.1	70.11	0.07	Positive	1	1	20.387	17110	3	1	
21	Cpd 21: C22 O...		C22 O10	34.29	Pass			423.9502		423.9491	-2.58	68.57	-1.09	Positive	1	1	9.341	1638	5	1	
15	Cpd 15: C25 H...		C25 H13 N...	33.53	Pass			733.0133		733.0134	0.1	67.06	0.07	Positive	1	1	21.999	4609	2	1	

Secondary metabolite identification for 26 Entities unic J5:

J5 semble une étape cruciale dans la croissance de Phaeodactylum on détecte 26 composés spécifiques à cette étapes dont:

Best Know: 9/926

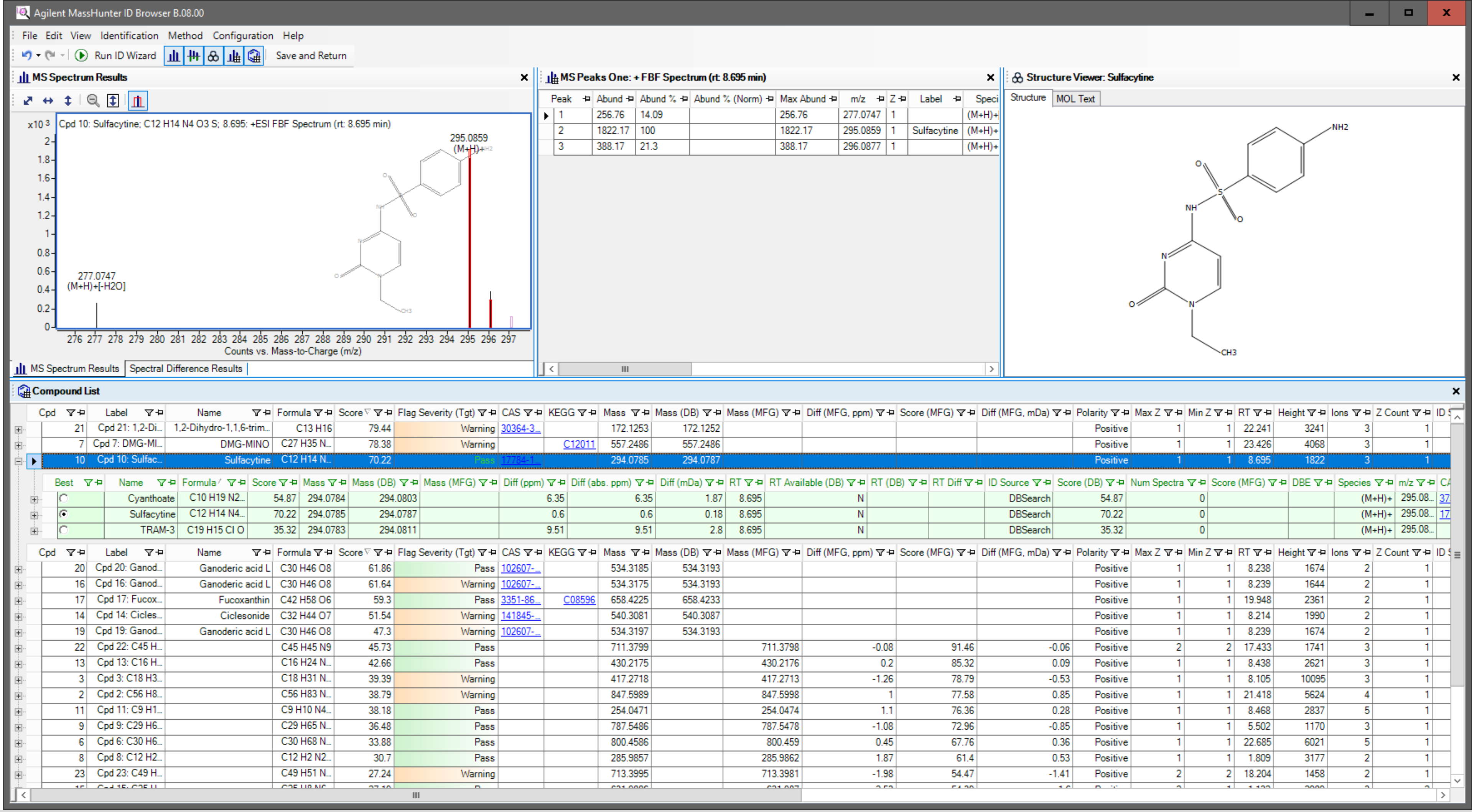


Cpd 12: Salicylanilide; C13 H11 N O2; 9.341: +ESI FBF Spectrum (rt: 9.341 min)

MS Peaks One: + FBF Spectrum (rt: 9.341 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Species	Clu
1	12433.66	100		12433.66	236.0669	1	Salicylanilide	(M+Na)+	1
2	2258.22	18.16		2258.22	237.072	1		(M+Na)+	1
3	199.88	1.61		199.88	238.0763	1		(M+Na)+	1

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT
12	Cpd 12: Salicyl...	Salicylanilide	C13 H11 N...	87.84	Pass	87-17-2	C18915	213.078	213.079					Positive	1	1	9.341
7	Cpd 7: Methyl 3...	Methyl 3-(2,3-dih...	C13 H18 O5	86.17	Pass	117176-...		254.1157	254.1154					Positive	1	1	8.471
5	Cpd 5: Talarom...	Talaromycin A	C12 H22 O4	86.12	Pass	83720-1...		230.1517	230.1518					Positive	1	1	9.29
13	Cpd 13: 3-oxo-...	3-oxo-dodecanoi...	C12 H22 O3	84.12	Pass			214.1577	214.1569					Positive	1	1	8.50
16	Cpd 16: Ferimz...	Ferimzone	C15 H18 N4	83.31	Pass	89269-6...	C18579	254.1524	254.1531					Positive	1	1	11.93
14	Cpd 14: (Z)-3-P...	(Z)-3-Phenyl-2-p...	C9 H8 O	83.05	Pass	57194-6...		132.0581	132.0575					Positive	1	1	9.34
10	Cpd 10: L-Ment...	L-Menthyl aceto...	C14 H24 O3	80.06	Pass	59557-0...		240.1713	240.1725					Positive	1	1	9.01
18	Cpd 18: Ellagic...	Ellagic acid	C14 H6 O8	73.63	Pass	476-66-4	C10788	302.0079	302.0063					Positive	1	1	9.341
20	Cpd 20: Gamm...	Gamma-glutamy...	C11 H21 N...	71.57	Warning			259.1552	259.1532					Positive	1	1	10.83
6	Cpd 6: Arachid...	Arachidonoyl Eth...	C22 H37 N...	65.85	Pass	94421-6...	C11695	347.281	347.2824					Positive	1	1	20.19
26	Cpd 26: 6-dem...	6-demethylgrise...	C16 H15 Cl...	42.2	Pass	20168-8...		338.0583	338.0557					Positive	1	1	6.99
4	Cpd 4: C24 N...		C24 N O27	42.19	Pass			733.865		733.8658	1.04	84.39	0.76	Positive	1	1	5.49
19	Cpd 19: C15 N...		C15 N2 O15	40.76	Pass			447.93		447.9299	-0.22	81.53	-0.1	Positive	1	1	9.341
8	Cpd 8: C20 H1...		C20 H12 N...	39.7	Pass			338.1042		338.1042	0.05	79.39	0.02	Positive	1	1	10.58
22	Cpd 22: C26 H...		C26 H8 N8...	39.02	Pass			512.0622		512.0618	-0.77	78.04	-0.39	Positive	1	1	13.00
25	Cpd 25: C13 H...		C13 H10 N...	37.62	Pass			422.0564		422.0571	1.49	75.25	0.63	Positive	1	1	10.58
24	Cpd 24: C14 H...		C14 H4 N2...	37.45	Pass			391.9774		391.9764	-2.58	74.91	-1.01	Positive	1	1	9.341
9	Cpd 9: C21 H1...		C21 H14 N...	37.24	Pass			512.1291		512.1292	0.12	74.47	0.06	Positive	2	1	9.35
2	Cpd 2: C28 H5...		C28 H50 N...	36.11	Warning			714.4376		714.4375	-0.21	72.22	-0.15	Positive	2	1	22.08
23	Cpd 23: C22 N...		C22 N O11	35.22	Pass			453.9472		453.9471	-0.22	70.44	-0.1	Positive	1	1	9.341
11	Cpd 11: C36 H...		C36 H65 N...	35.05	Pass			727.5333		727.5333	0.1	70.11	0.07	Positive	1	1	20.38
21	Cpd 21: C22 O...		C22 O10	34.29	Pass			423.9502		423.9491	-2.58	68.57	-1.09	Positive	1	1	9.341
15	Cpd 15: C25 H...		C25 H13 N...	33.53	Pass			733.0133		733.0134	0.1	67.06	0.07	Positive	1	1	21.99



Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Speci
1	256.76	14.09		256.76	277.0747	1		(M+H)+
2	1822.17	100		1822.17	295.0859	1	Sulfacytine	(M+H)+
3	388.17	21.3		388.17	296.0877	1		(M+H)+

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT	Height	Ions	Z Count
21	Cpd 21: 1,2-Di...	1,2-Dihydro-1,1,6-trim...	C13 H16	79.44	Warning	30364-3...		172.1253	172.1252					Positive	1	1	22.241	3241	3	1
7	Cpd 7: DMG-MI...	DMG-MINO	C27 H35 N...	78.38	Warning		C12011	557.2486	557.2486					Positive	1	1	23.426	4068	3	1
10	Cpd 10: Sulfac...	Sulfacytine	C12 H14 N...	70.22	Pass	17784-1...		294.0785	294.0787					Positive	1	1	8.695	1822	3	1

Best	Name	Formula	Score	Mass	Mass (DB)	Mass (MFG)	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	RT	RT Available (DB)	RT (DB)	RT Diff	ID Source	Score (DB)	Num Spectra	Score (MFG)	DBE	Species	m/z
○	Cyanthoate	C10 H19 N2...	54.87	294.0784	294.0803		6.35	6.35	1.87	8.695	N			DBSearch	54.87	0			(M+H)+	295.08...
●	Sulfacytine	C12 H14 N4...	70.22	294.0785	294.0787		0.6	0.6	0.18	8.695	N			DBSearch	70.22	0			(M+H)+	295.08...
○	TRAM-3	C19 H15 Cl O	35.32	294.0783	294.0811		9.51	9.51	2.8	8.695	N			DBSearch	35.32	0			(M+H)+	295.08...

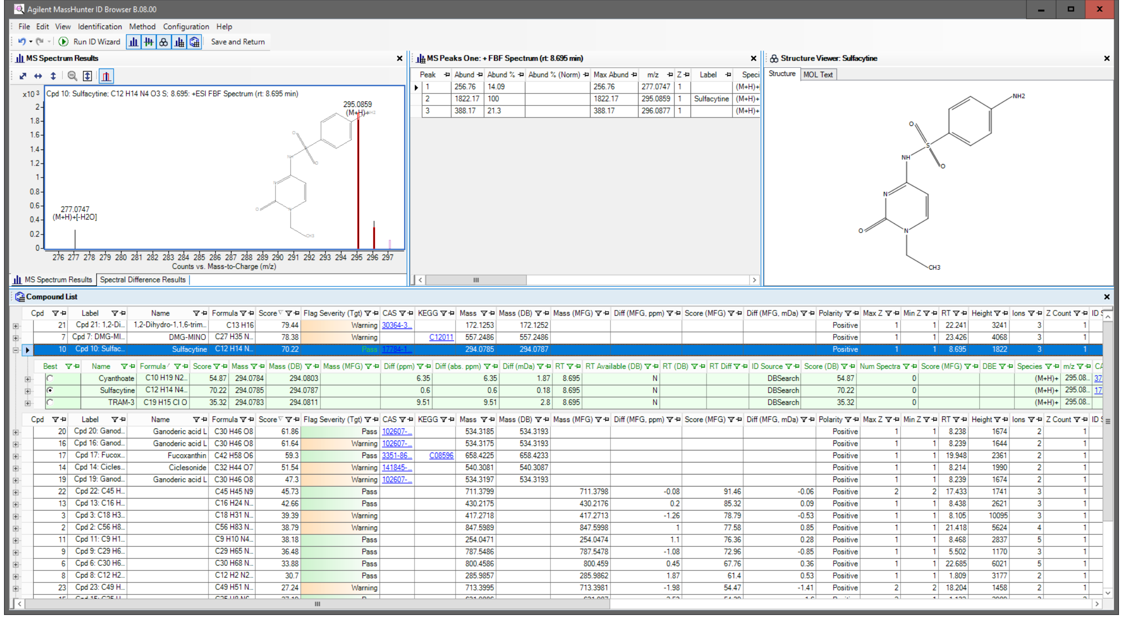
Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT	Height	Ions	Z Count
20	Cpd 20: Ganod...	Ganoderic acid L	C30 H46 O8	61.86	Pass	102607-...		534.3185	534.3193					Positive	1	1	8.238	1674	2	1
16	Cpd 16: Ganod...	Ganoderic acid L	C30 H46 O8	61.64	Warning	102607-...		534.3175	534.3193					Positive	1	1	8.239	1644	2	1
17	Cpd 17: Fucox...	Fucoxanthin	C42 H58 O6	59.3	Pass	3351-86...	C08596	658.4225	658.4233					Positive	1	1	19.948	2361	2	1
14	Cpd 14: Cicles...	Ciclesonide	C32 H44 O7	51.54	Warning	141845-...		540.3081	540.3087					Positive	1	1	8.214	1990	2	1
19	Cpd 19: Ganod...	Ganoderic acid L	C30 H46 O8	47.3	Warning	102607-...		534.3197	534.3193					Positive	1	1	8.239	1674	2	1
22	Cpd 22: C45 H...		C45 H45 N9	45.73	Pass			711.3799		711.3798	-0.08	91.46	-0.06	Positive	2	2	17.433	1741	3	1
13	Cpd 13: C16 H...		C16 H24 N...	42.66	Pass			430.2175		430.2176	0.2	85.32	0.09	Positive	1	1	8.438	2621	3	1
3	Cpd 3: C18 H3...		C18 H31 N...	39.39	Warning			417.2718		417.2713	-1.26	78.79	-0.53	Positive	1	1	8.105	10095	3	1
2	Cpd 2: C56 H8...		C56 H83 N...	38.79	Warning			847.5989		847.5998	1	77.58	0.85	Positive	1	1	21.418	5624	4	1
11	Cpd 11: C9 H1...		C9 H10 N4...	38.18	Pass			254.0471		254.0474	1.1	76.36	0.28	Positive	1	1	8.468	2837	5	1
9	Cpd 9: C29 H6...		C29 H65 N...	36.48	Pass			787.5486		787.5478	-1.08	72.96	-0.85	Positive	1	1	5.502	1170	3	1
6	Cpd 6: C30 H6...		C30 H68 N...	33.88	Pass			800.4586		800.459	0.45	67.76	0.36	Positive	1	1	22.685	6021	5	1
8	Cpd 8: C12 H2...		C12 H2 N2...	30.7	Pass			285.9857		285.9862	1.87	61.4	0.53	Positive	1	1	1.809	3177	2	1
23	Cpd 23: C49 H...		C49 H51 N...	27.24	Warning			713.3995		713.3981	-1.98	54.47	-1.41	Positive	2	2	18.204	1458	2	1

Secondary metabolite identification for 23 Entities unic J6:

J6 semble être une autre étape cruciale dans la croissance de Phaeodactylum proche de J5 et pour laquelle on détecte 23 composés spécifiques mais dont l’identification se résume à 1 ou 2 composés pour lequel l’identification donne un score acceptable

Best Know: 2/23

- Cpd 10: Sulfacytine; $C_{12}H_{14}N_4O_3S$ @8.695 Score: 70.22



MS Peaks One: + FBF Spectrum (rt: 8.695 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Speci
1	256.76	14.09		256.76	277.0747	1		(M+H)+
2	1822.17	100		1822.17	295.0859	1	Sulfacytine	(M+H)+
3	388.17	21.3		388.17	296.0877	1		(M+H)+

Compound List

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT	Height	Ions	Z Count
21	Cpd 21: 1,2-Di...	1,2-Dihydro-1,1,6-trim...	C13 H16	79.44	Warning	30364-3...		172.1253	172.1252					Positive	1	1	22.241	3241	3	1
7	Cpd 7: DMG-MI...	DMG-MINO	C27 H35 N...	78.38	Warning		C12011	557.2486	557.2486					Positive	1	1	23.426	4068	3	1
10	Cpd 10: Sulfac...	Sulfacytine	C12 H14 N...	70.22	Pass	17784-1...		294.0785	294.0787					Positive	1	1	8.695	1822	3	1

Best	Name	Formula	Score	Mass	Mass (DB)	Mass (MFG)	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	RT	RT Available (DB)	RT (DB)	RT Diff	ID Source	Score (DB)	Num Spectra	Score (MFG)	DBE	Species	m/z
○	Cyanthoate	C10 H19 N2...	54.87	294.0784	294.0803		6.35	6.35	1.87	8.695	N			DBSearch	54.87	0			(M+H)+	295.08...
●	Sulfacytine	C12 H14 N4...	70.22	294.0785	294.0787		0.6	0.6	0.18	8.695	N			DBSearch	70.22	0			(M+H)+	295.08...
○	TRAM-3	C19 H15 Cl O	35.32	294.0783	294.0811		9.51	9.51	2.8	8.695	N			DBSearch	35.32	0			(M+H)+	295.08...

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	RT	Height	Ions	Z Count
20	Cpd 20: Ganod...	Ganoderic acid L	C30 H46 O8	61.86	Pass	102607-...		534.3185	534.3193					Positive	1	1	8.238	1674	2	1
16	Cpd 16: Ganod...	Ganoderic acid L	C30 H46 O8	61.64	Warning	102607-...		534.3175	534.3193					Positive	1	1	8.239	1644	2	1
17	Cpd 17: Fucox...	Fucoxanthin	C42 H58 O6	59.3	Pass	3351-86...	C08596	658.4225	658.4233					Positive	1	1	19.948	2361	2	1
14	Cpd 14: Cicles...	Ciclesonide	C32 H44 O7	51.54	Warning	141845-...		540.3081	540.3087					Positive	1	1	8.214	1990	2	1
19	Cpd 19: Ganod...	Ganoderic acid L	C30 H46 O8	47.3	Warning	102607-...		534.3197	534.3193					Positive	1	1	8.239	1674	2	1
22	Cpd 22: C45 H...		C45 H45 N9	45.73	Pass			711.3799		711.3798	-0.08	91.46	-0.06	Positive	2	2	17.433	1741	3	1
13	Cpd 13: C16 H...		C16 H24 N...	42.66	Pass			430.2175		430.2176	0.2	85.32	0.09	Positive	1	1	8.438	2621	3	1
3	Cpd 3: C18 H3...		C18 H31 N...	39.39	Warning			417.2718		417.2713	-1.26	78.79	-0.53	Positive	1	1	8.105	10095	3	1
2	Cpd 2: C56 H8...		C56 H83 N...	38.79	Warning			847.5989		847.5998	1	77.58	0.85	Positive	1	1	21.418	5624	4	1
11	Cpd 11: C9 H1...		C9 H10 N4...	38.18	Pass			254.0471		254.0474	1.1	76.36	0.28	Positive	1	1	8.468	2837	5	1
9	Cpd 9: C29 H6...		C29 H65 N...	36.48	Pass			787.5486		787.5478	-1.08	72.96	-0.85	Positive	1	1	5.502	1170	3	1
6	Cpd 6: C30 H6...		C30 H68 N...	33.88	Pass			800.4586		800.459	0.45	67.76	0.36	Positive	1	1	22.685	6021	5	1
8	Cpd 8: C12 H2...		C12 H2 N2...	30.7	Pass			285.9857		285.9862	1.87	61.4	0.53	Positive	1	1	1.809	3177	2	1
23	Cpd 23: C49 H...		C49 H51 N...	27.24	Warning			713.3995		713.3981	-1.98	54.47	-1.41	Positive	2	2	18.204	1458	2	1

Secondary metabolite identification for 23 Entities unic J6:

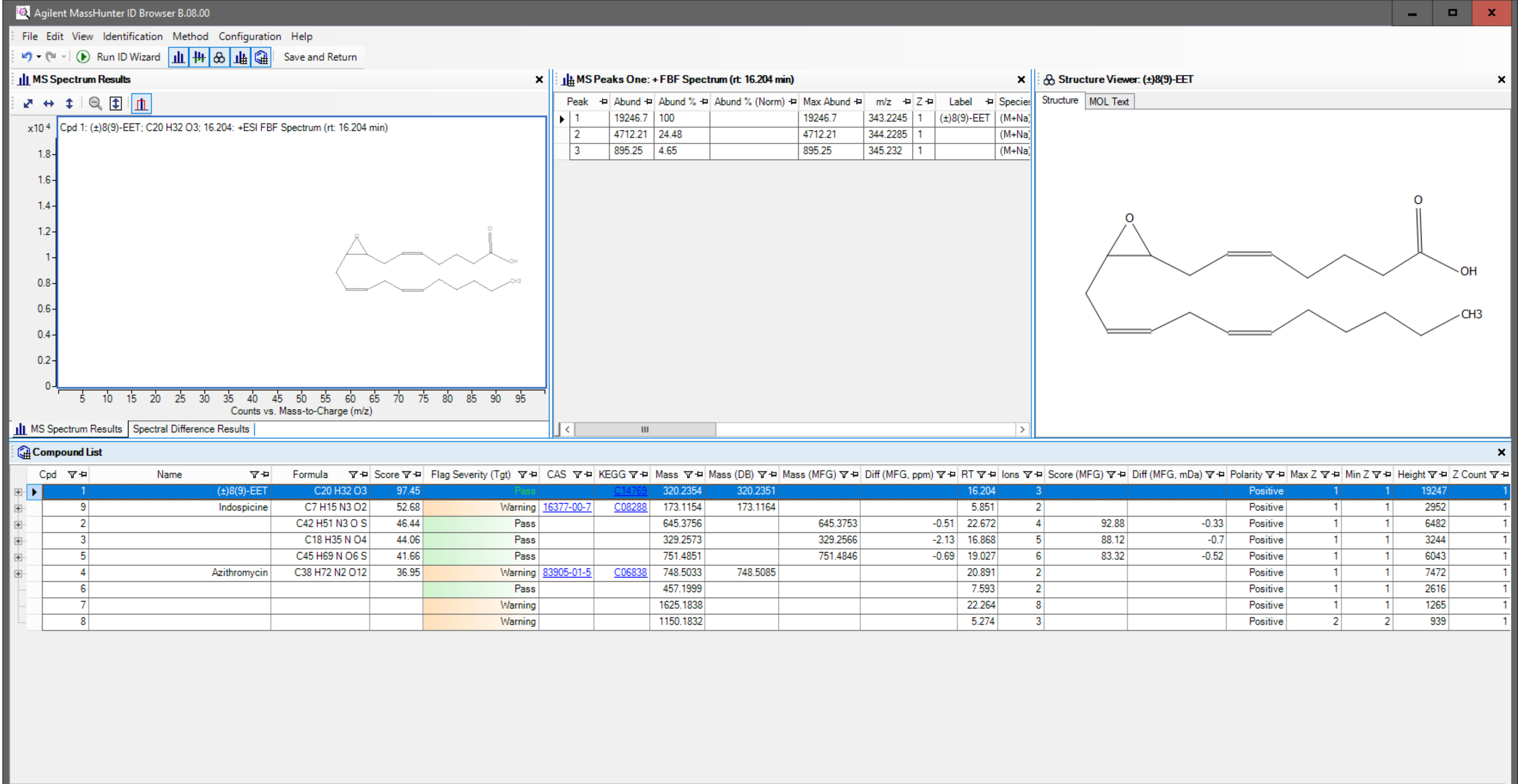
Best Know: 2/23

- Cpd 10: Sulfacytine; $C_{12}H_{14}N_4O_3S$ @8.695 Score: 70.22

Sulfacytine is a member of benzenes and a sulfonamide. Sulfacytine is a short-acting, broad-spectrum sulfonamide and a synthetic analog of para-aminobenzoic acid (PABA) with bacteriostatic property. Sulfacytine competes with PABA for the bacterial enzyme dihydropteroate synthase, thereby preventing the incorporation of PABA into dihydrofolic acid, the immediate precursor of folic acid. This leads to an inhibition of bacterial folic acid synthesis and de novo synthesis of purines and pyrimidines, ultimately resulting in cell growth arrest and cell death

Cpd 20: Ganoderic acid L; $C_{30}H_{46}O_8$ @8.238 Score: 61.86

There seems to exist certain relationship between specific Ganoderic acid production (ie content) and DOxygenT level. Further experiments were conducted to explore this potential Relationship (YJ Tang et al. 2003)



MS Peaks One: + FBF Spectrum (rt: 16.204 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Species
1	19246.7	100		19246.7	343.2245	1	(±)8(9)-EET	(M+Na)
2	4712.21	24.48		4712.21	344.2285	1		(M+Na)
3	895.25	4.65		895.25	345.232	1		(M+Na)

Compound List

Cpd	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	RT	Ions	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	Height	Z Count
1	(±)8(9)-EET	C20 H32 O3	97.45	Pass		C14769	320.2354	320.2351			16.204	3			Positive	1	1	19247	1
9	Indospicine	C7 H15 N3 O2	52.68	Warning	16377-00-7	C08288	173.1154	173.1164			5.851	2			Positive	1	1	2952	1
2		C42 H51 N3 O S	46.44	Pass			645.3756		645.3753	-0.51	22.672	4	92.88	-0.33	Positive	1	1	6482	1
3		C18 H35 N O4	44.06	Pass			329.2573		329.2566	-2.13	16.868	5	88.12	-0.7	Positive	1	1	3244	1
5		C45 H69 N O6 S	41.66	Pass			751.4851		751.4846	-0.69	19.027	6	83.32	-0.52	Positive	1	1	6043	1
4	Azithromycin	C38 H72 N2 O12	36.95	Warning	83905-01-5	C06838	748.5033	748.5085			20.891	2			Positive	1	1	7472	1
6				Pass			457.1999				7.593	2			Positive	1	1	2616	1
7				Warning			1625.1838				22.264	8			Positive	1	1	1265	1
8				Warning			1150.1832				5.274	3			Positive	2	2	939	1

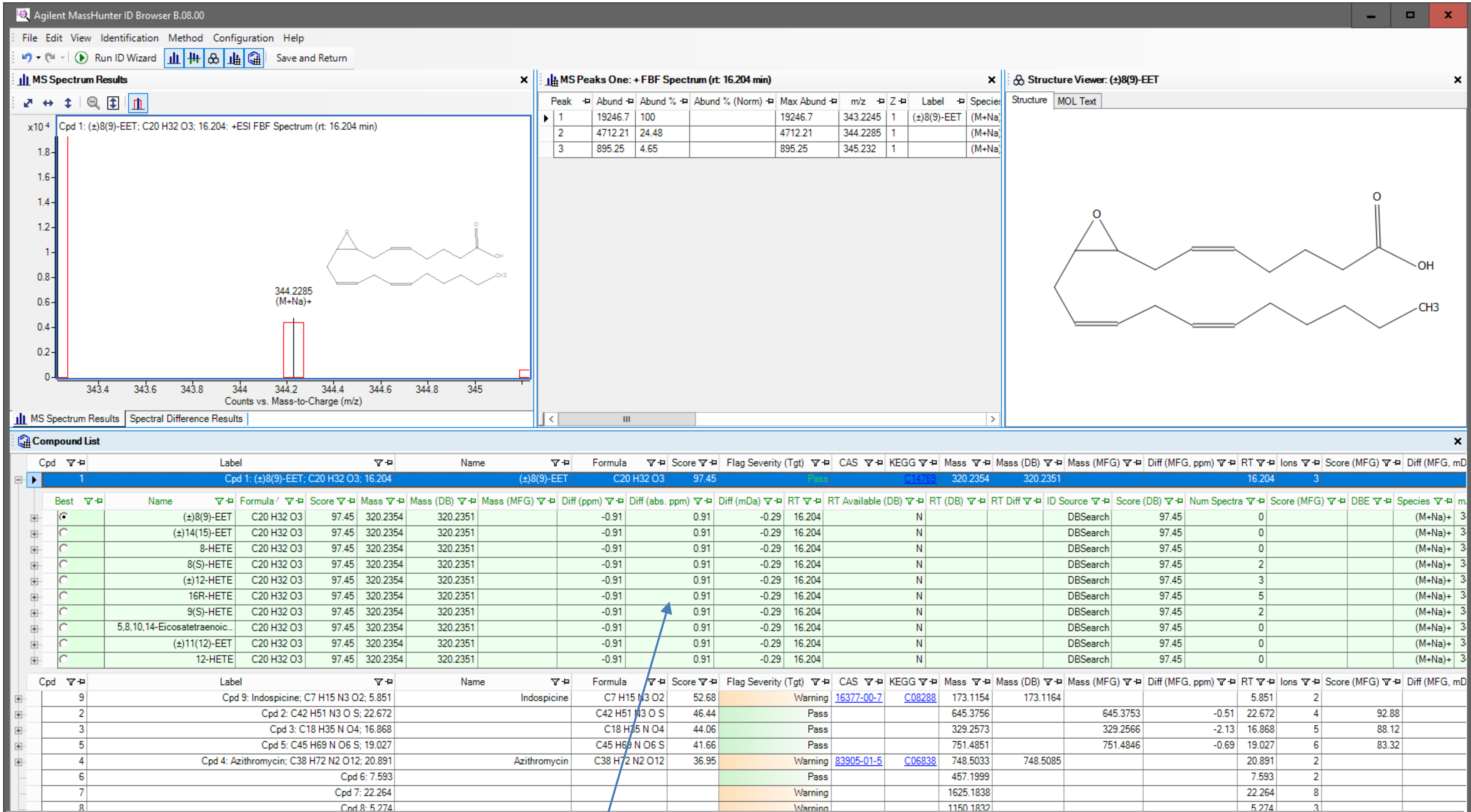
Secondary metabolite identification for 9 Entities unic J8

- Best know: 1/8

Oxylipin : eicosatetraenoic acid (5-HETE) ou bien 10 autres putatifs compounds visibles dans la slide suivante dans l’onglet en vert,

Cpd 1: (±)8(9)-EET; ; C20H32O3@16.204 score :97.45

Issu de: Arachidonic acid metabolism



Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label	Specie
1	19246.7	100		19246.7	343.2245	1	(±)8(9)-EET	(M+Na)
2	4712.21	24.48		4712.21	344.2285	1		(M+Na)
3	895.25	4.65		895.25	345.232	1		(M+Na)

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	RT	Ions	Score (MFG)	Diff (MFG, mD
1	Cpd 1: (±)8(9)-EET; C20 H32 O3; 16.204	(±)8(9)-EET	C20 H32 O3	97.45	Pass		C14769	320.2354	320.2351			16.204	3		

Best	Name	Formula	Score	Mass	Mass (DB)	Mass (MFG)	Diff (ppm)	Diff (abs. ppm)	Diff (mDa)	RT	RT Available (DB)	RT (DB)	RT Diff	ID Source	Score (DB)	Num Spectra	Score (MFG)	DBE	Species
●	(±)8(9)-EET	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	0			(M+Na)+
○	(±)14(15)-EET	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	0			(M+Na)+
○	8-HETE	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	0			(M+Na)+
○	8(S)-HETE	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	2			(M+Na)+
○	(±)12-HETE	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	3			(M+Na)+
○	16R-HETE	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	5			(M+Na)+
○	9(S)-HETE	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	2			(M+Na)+
○	5,8,10,14-Eicosatetraenoic...	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	0			(M+Na)+
○	(±)11(12)-EET	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	0			(M+Na)+
○	12-HETE	C20 H32 O3	97.45	320.2354	320.2351		-0.91	0.91	-0.29	16.204	N			DBSearch	97.45	0			(M+Na)+

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	RT	Ions	Score (MFG)	Diff (MFG, mD
9	Cpd 9: Indospicine; C7 H15 N3 O2; 5.851	Indospicine	C7 H15 N3 O2	52.68	Warning	16377-00-7	C08288	173.1154	173.1164			5.851	2		
2	Cpd 2: C42 H51 N3 O S; 22.672		C42 H51 N3 O S	46.44	Pass			645.3756		645.3753	-0.51	22.672	4	92.88	
3	Cpd 3: C18 H35 N O4; 16.868		C18 H35 N O4	44.06	Pass			329.2573		329.2566	-2.13	16.868	5	88.12	
5	Cpd 5: C45 H69 N O6 S; 19.027		C45 H69 N O6 S	41.66	Pass			751.4851		751.4846	-0.69	19.027	6	83.32	
4	Cpd 4: Azithromycin; C38 H72 N2 O12; 20.891	Azithromycin	C38 H72 N2 O12	36.95	Warning	83905-01-5	C06838	748.5033	748.5085			20.891	2		
6	Cpd 6: 7.593				Pass			457.1999				7.593	2		
7	Cpd 7: 22.264				Warning			1625.1838				22.264	8		
8	Cpd 8: 5.274				Warning			1150.1832				5.274	3		

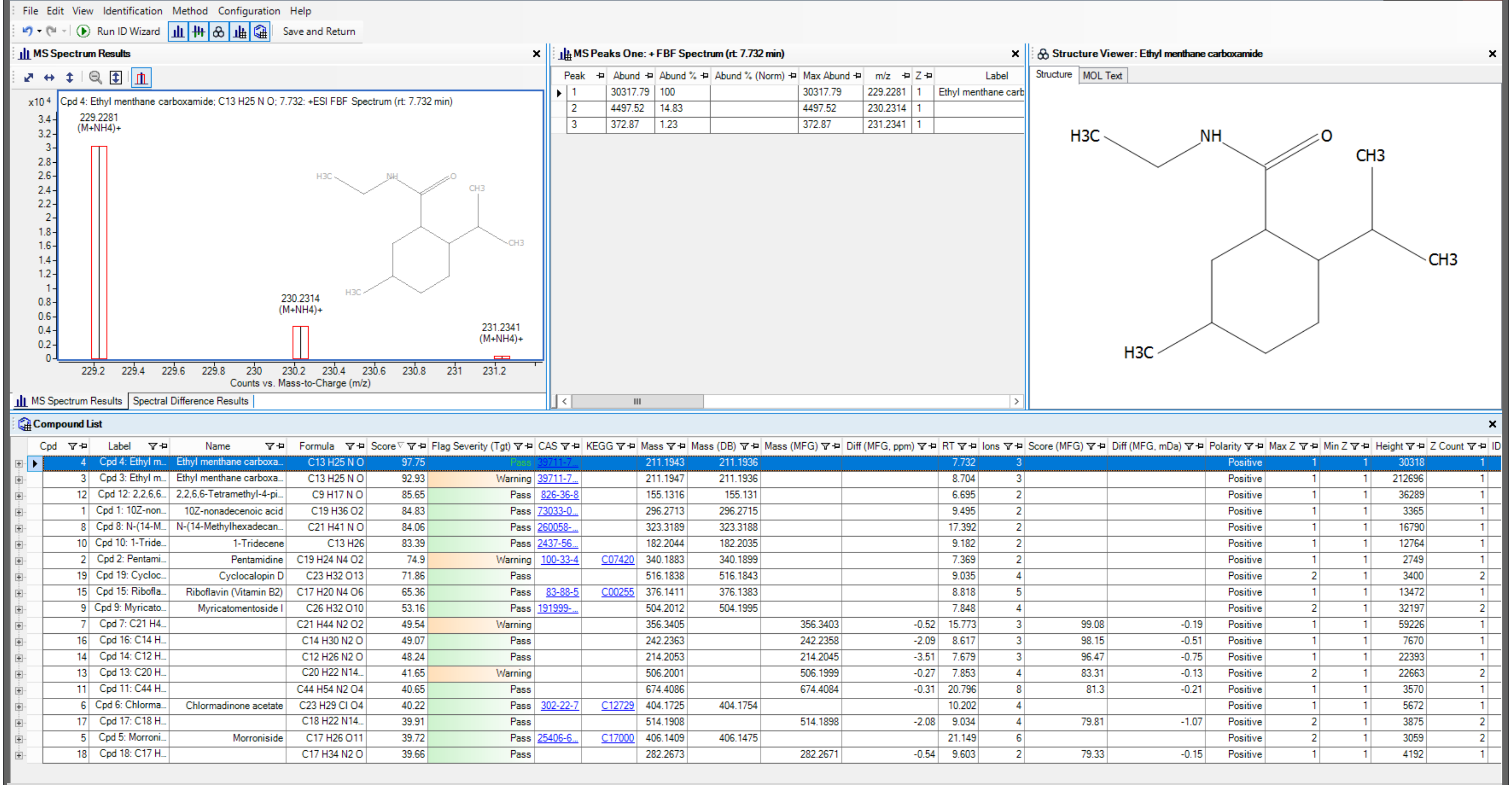
Secondary metabolite identification for 9 Entities unic J8

- Best know: 1/8

Oxylipin : eicosatetraenoic acid (5-HETE) ou bien 10 autres putatifs compounds visibles dans la slide suivante dans l'onglet en vert,

Cpd 1: (±)8(9)-EET; C20H32O3@16.204 score :97.45

Issu de: Arachidonic acid metabolism

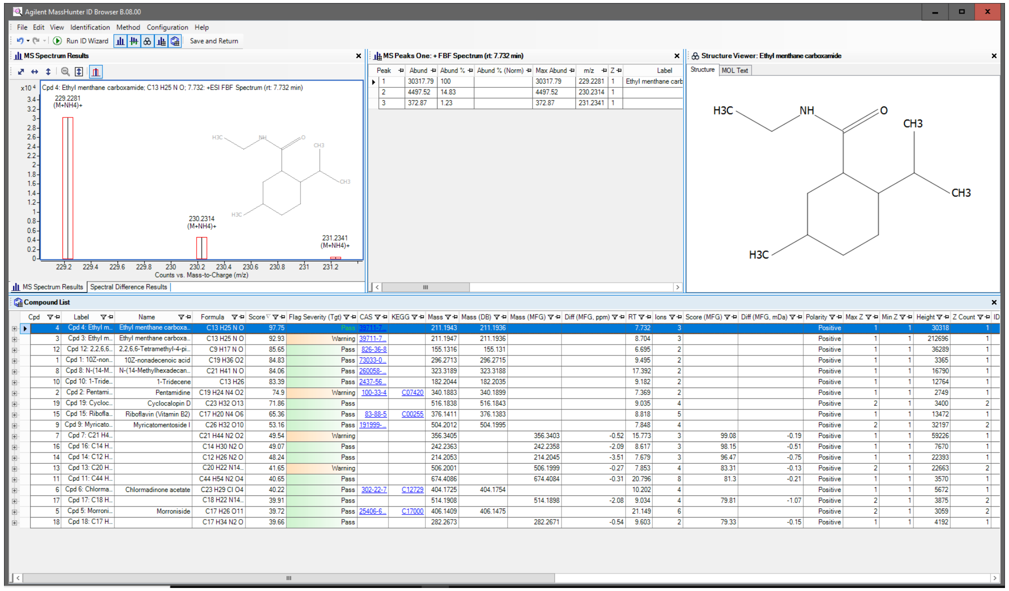


Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label
1	30317.79	100		30317.79	229.2281	1	Ethyl menthane carb
2	4497.52	14.83		4497.52	230.2314	1	
3	372.87	1.23		372.87	231.2341	1	

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	RT	Ions	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	Height	Z Count	ID
4	Cpd 4: Ethyl m...	Ethyl menthane carboxa...	C13 H25 N O	97.75	Pass	39711-7...		211.1943	211.1936			7.732	3			Positive	1	1	30318	1	
3	Cpd 3: Ethyl m...	Ethyl menthane carboxa...	C13 H25 N O	92.93	Warning	39711-7...		211.1947	211.1936			8.704	3			Positive	1	1	212696	1	
12	Cpd 12: 2,2,6,6...	2,2,6,6-Tetramethyl-4-pi...	C9 H17 N O	85.65	Pass	826-36-8		155.1316	155.131			6.695	2			Positive	1	1	36289	1	
1	Cpd 1: 10Z-non...	10Z-nonadecenoic acid	C19 H36 O2	84.83	Pass	73033-0...		296.2713	296.2715			9.495	2			Positive	1	1	3365	1	
8	Cpd 8: N-(14-M...	N-(14-Methylhexadecan...	C21 H41 N O	84.06	Pass	260058-...		323.3189	323.3188			17.392	2			Positive	1	1	16790	1	
10	Cpd 10: 1-Tride...	1-Tridecene	C13 H26	83.39	Pass	2437-56...		182.2044	182.2035			9.182	2			Positive	1	1	12764	1	
2	Cpd 2: Pentami...	Pentamidine	C19 H24 N4 O2	74.9	Warning	100-33-4	C07420	340.1883	340.1899			7.369	2			Positive	1	1	2749	1	
19	Cpd 19: Cycloc...	Cyclocalopin D	C23 H32 O13	71.86	Pass			516.1838	516.1843			9.035	4			Positive	2	1	3400	2	
15	Cpd 15: Ribofla...	Riboflavin (Vitamin B2)	C17 H20 N4 O6	65.36	Pass	83-88-5	C00255	376.1411	376.1383			8.818	5			Positive	1	1	13472	1	
9	Cpd 9: Myricato...	Myricatomentoside I	C26 H32 O10	53.16	Pass	191999-...		504.2012	504.1995			7.848	4			Positive	2	1	32197	2	
7	Cpd 7: C21 H4...		C21 H44 N2 O2	49.54	Warning			356.3405		356.3403	-0.52	15.773	3	99.08	-0.19	Positive	1	1	59226	1	
16	Cpd 16: C14 H...		C14 H30 N2 O	49.07	Pass			242.2363		242.2358	-2.09	8.617	3	98.15	-0.51	Positive	1	1	7670	1	
14	Cpd 14: C12 H...		C12 H26 N2 O	48.24	Pass			214.2053		214.2045	-3.51	7.679	3	96.47	-0.75	Positive	1	1	22393	1	
13	Cpd 13: C20 H...		C20 H22 N14...	41.65	Warning			506.2001		506.1999	-0.27	7.853	4	83.31	-0.13	Positive	2	1	22663	2	
11	Cpd 11: C44 H...		C44 H54 N2 O4	40.65	Pass			674.4086		674.4084	-0.31	20.796	8	81.3	-0.21	Positive	1	1	3570	1	
6	Cpd 6: Chlorma...	Chlormadinone acetate	C23 H29 Cl O4	40.22	Pass	302-22-7	C12729	404.1725	404.1754			10.202	4			Positive	1	1	5672	1	
17	Cpd 17: C18 H...		C18 H22 N14...	39.91	Pass			514.1908		514.1898	-2.08	9.034	4	79.81	-1.07	Positive	2	1	3875	2	
5	Cpd 5: Morroni...	Morroniside	C17 H26 O11	39.72	Pass	25406-6...	C17000	406.1409	406.1475			21.149	6			Positive	2	1	3059	2	
18	Cpd 18: C17 H...		C17 H34 N2 O	39.66	Pass			282.2673		282.2671	-0.54	9.603	2	79.33	-0.15	Positive	1	1	4192	1	

Secondary metabolite identification for 19 Entities unic Jmax de 10 à 11

- Best know: 5/19
- Cpd 4: Ethyl menthane carboxamide; C13H25NO @7.732 Score :97.75
- Cpd 12: 2,2,6,6-Tetramethyl-4-piperidinone; C9H17NO @6.695 Score: 85.65
- Cpd 1: 10Z-nonadecenoic acid; C19H36O2 @ 9.495 Score: 84.83
- Cpd 8: N-(14-Methylhexadecanoyl)pyrrolidine; C21H41NO @17.392 Score: 84.06
- Cpd 10: 1-Tridecene; C13 H26 @9.182 Score: 83.39



MS Peaks One: + FBF Spectrum (rt: 7.732 min)

Peak	Abund	Abund %	Abund % (Norm)	Max Abund	m/z	Z	Label
1	30317.79	100		30317.79	229.2281	1	Ethyl menthane carb
2	4497.52	14.83		4497.52	230.2314	1	
3	372.87	1.23		372.87	231.2341	1	

Compound List

Cpd	Label	Name	Formula	Score	Flag Severity (Tgt)	CAS	KEGG	Mass	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	RT	Ions	Score (MFG)	Diff (MFG, mDa)	Polarity	Max Z	Min Z	Height	Z Count
4	Cpd 4: Ethyl m...	Ethyl menthane carboxa...	C13 H25 N O	97.75	Pass	39711-7...		211.1943	211.1936			7.732	3			Positive	1	1	30318	1
3	Cpd 3: Ethyl m...	Ethyl menthane carboxa...	C13 H25 N O	92.93	Warning	39711-7...		211.1947	211.1936			8.704	3			Positive	1	1	212696	1
12	Cpd 12: 2,2,6,6...	2,2,6,6-Tetramethyl-4-pi...	C9 H17 N O	85.65	Pass	826-36-8		155.1316	155.131			6.695	2			Positive	1	1	36289	1
1	Cpd 1: 10Z-non...	10Z-nonadecenoic acid	C19 H36 O2	84.83	Pass	73033-0...		296.2713	296.2715			9.495	2			Positive	1	1	3365	1
8	Cpd 8: N-(14-M...	N-(14-Methylhexadecan...	C21 H41 N O	84.06	Pass	260058-...		323.3189	323.3188			17.392	2			Positive	1	1	16790	1
10	Cpd 10: 1-Tride...	1-Tridecene	C13 H26	83.39	Pass	2437-56...		182.2044	182.2035			9.182	2			Positive	1	1	12764	1
2	Cpd 2: Pentami...	Pentamidine	C19 H24 N4 O2	74.9	Warning	100-33-4	C07420	340.1883	340.1899			7.369	2			Positive	1	1	2749	1
19	Cpd 19: Cycloc...	Cyclocalopin D	C23 H32 O13	71.86	Pass			516.1838	516.1843			9.035	4			Positive	2	1	3400	2
15	Cpd 15: Ribofla...	Riboflavin (Vitamin B2)	C17 H20 N4 O6	65.36	Pass	83-88-5	C00255	376.1411	376.1383			8.818	5			Positive	1	1	13472	1
9	Cpd 9: Myricato...	Myricatomentoside I	C26 H32 O10	53.16	Pass	191999-...		504.2012	504.1995			7.848	4			Positive	2	1	32197	2
7	Cpd 7: C21 H4...		C21 H44 N2 O2	49.54	Warning			356.3405		356.3403	-0.52	15.773	3	99.08	-0.19	Positive	1	1	59226	1
16	Cpd 16: C14 H...		C14 H30 N2 O	49.07	Pass			242.2363		242.2358	-2.09	8.617	3	98.15	-0.51	Positive	1	1	7670	1
14	Cpd 14: C12 H...		C12 H26 N2 O	48.24	Pass			214.2053		214.2045	-3.51	7.679	3	96.47	-0.75	Positive	1	1	22393	1
13	Cpd 13: C20 H...		C20 H22 N14...	41.65	Warning			506.2001		506.1999	-0.27	7.853	4	83.31	-0.13	Positive	2	1	22663	2
11	Cpd 11: C44 H...		C44 H54 N2 O4	40.65	Pass			674.4086		674.4084	-0.31	20.796	8	81.3	-0.21	Positive	1	1	3570	1
6	Cpd 6: Chlorma...	Chlormadinone acetate	C23 H29 Cl O4	40.22	Pass	302-22-7	C12729	404.1725	404.1754			10.202	4			Positive	1	1	5672	1
17	Cpd 17: C18 H...		C18 H22 N14...	39.91	Pass			514.1908		514.1898	-2.08	9.034	4	79.81	-1.07	Positive	2	1	3875	2
5	Cpd 5: Morroni...	Morroniside	C17 H26 O11	39.72	Pass	25406-6...	C17000	406.1409	406.1475			21.149	6			Positive	2	1	3059	2
18	Cpd 18: C17 H...		C17 H34 N2 O	39.66	Pass			282.2673		282.2671	-0.54	9.603	2	79.33	-0.15	Positive	1	1	4192	1

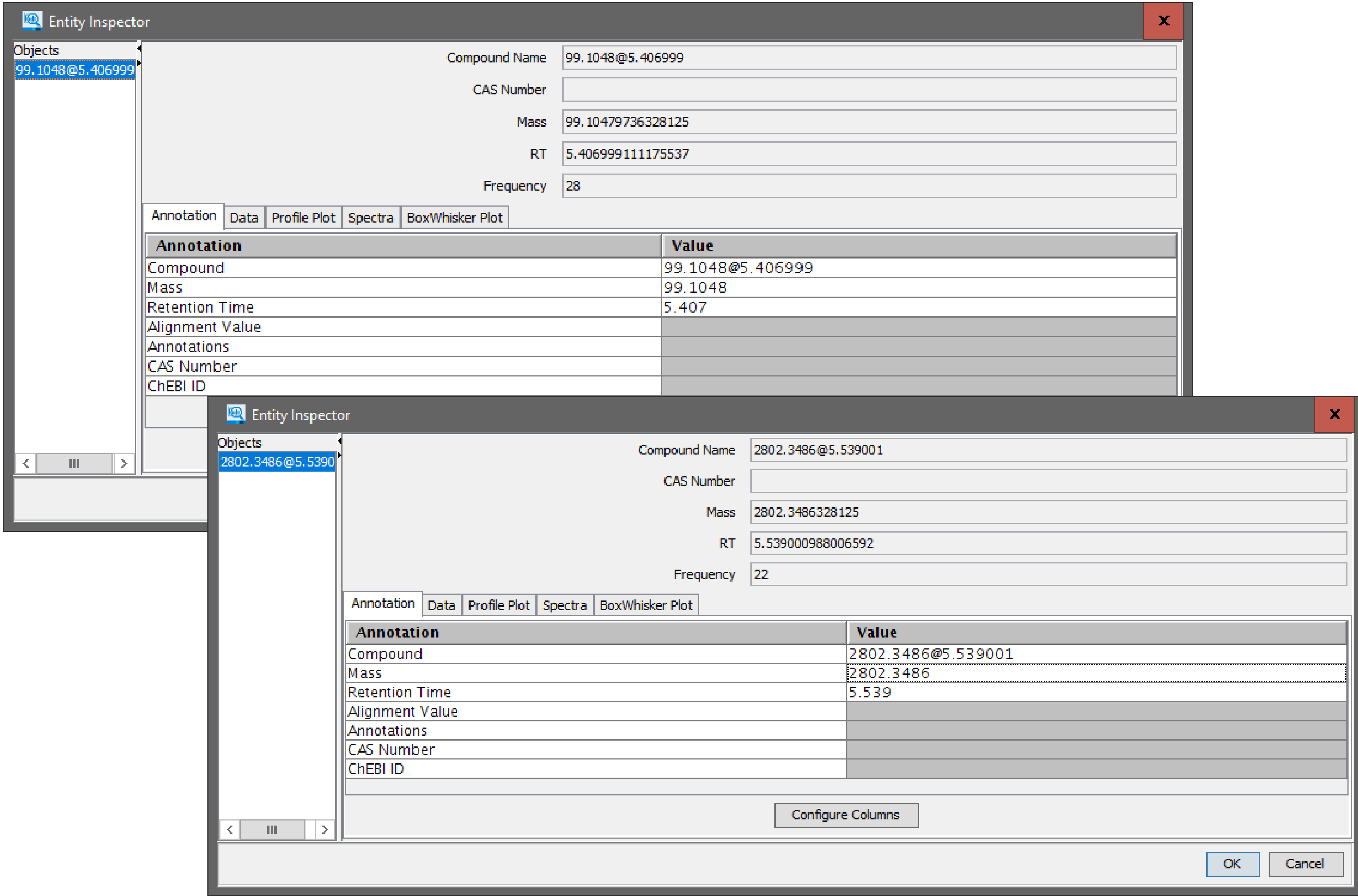
Secondary metabolite identification for 19 Entities unic Jmax de 10 à 11

- Best know: 5/19
- Cpd 4: Ethyl menthane carboxamide; $C_{13}H_{25}NO$ @7.732 Score :97.75
- Cpd 12: 2,2,6,6-Tetramethyl-4-piperidinone; $C_9H_{17}NO$ @6.695 Score: 85.65
- Cpd 1: 10Z-nonadecenoic acid; $C_{19}H_{36}O_2$ @ 9.495 Score: 84.83

→*Inhibitors of oleamide hydrolase*

- Cpd 8: N-(14-Methylhexadecanoyl)pyrrolidine; $C_{21}H_{41}NO$ @17.392 Score: 84.06
- Cpd 10: 1-Tridecene; $C_{13}H_{26}$ @9.182 Score: 83.39

SUITE
avec pour info pour Benoit :
le plus petit métabolite analysé et le plus grand.



Entity Inspector

Objects: 99.1048@5.406999

Compound Name	99.1048@5.406999
CAS Number	
Mass	99.10479736328125
RT	5.406999111175537
Frequency	28

Annotation	Value
Compound	99.1048@5.406999
Mass	99.1048
Retention Time	5.407
Alignment Value	
Annotations	
CAS Number	
ChEBI ID	

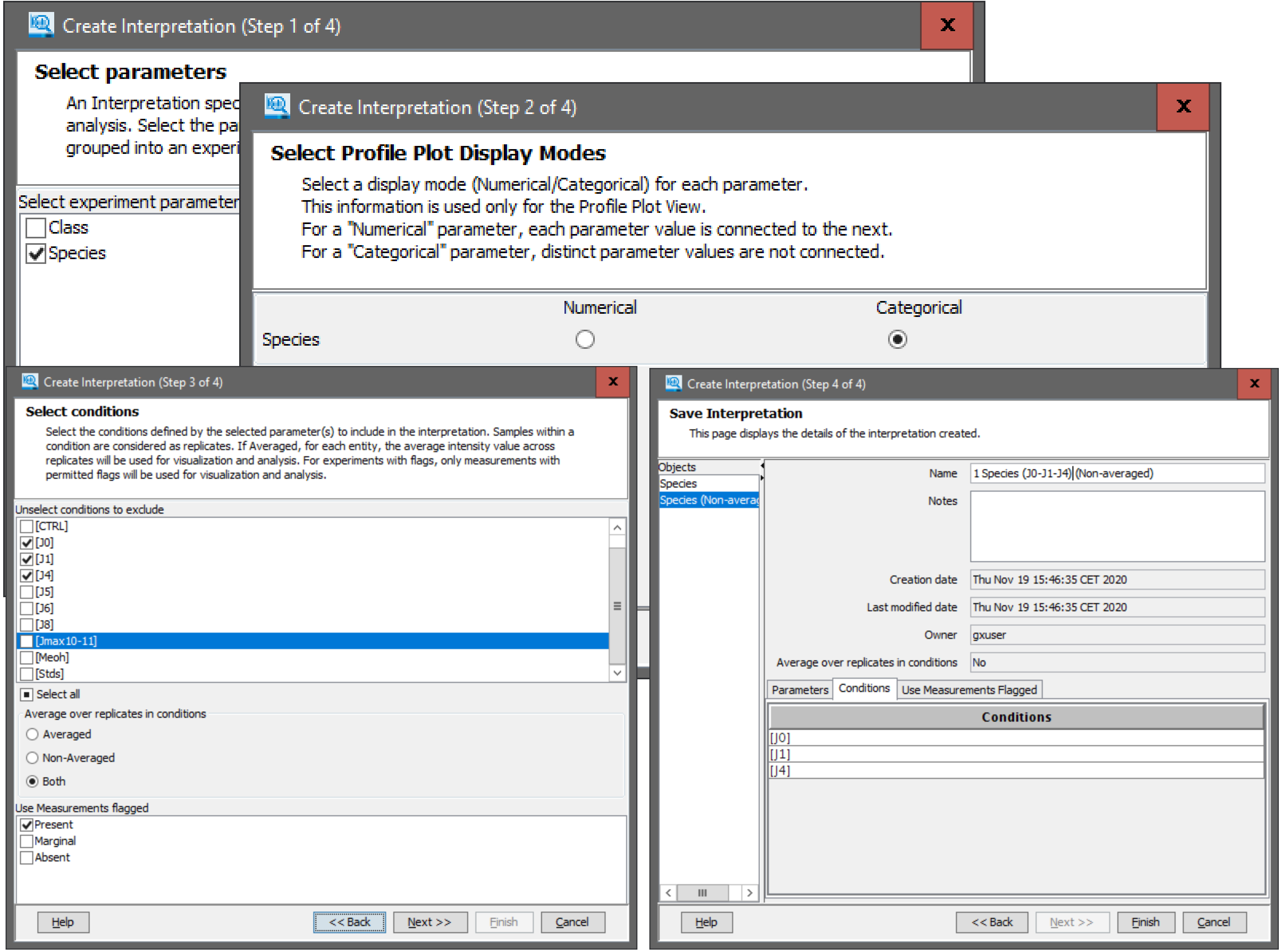
Entity Inspector

Objects: 2802.3486@5.5390

Compound Name	2802.3486@5.539001
CAS Number	
Mass	2802.3486328125
RT	5.539000988006592
Frequency	22

Annotation	Value
Compound	2802.3486@5.539001
Mass	2802.3486
Retention Time	5.539
Alignment Value	
Annotations	
CAS Number	
ChEBI ID	

Créations des nouvelles interprétations



Create Interpretation (Step 1 of 4)

Select parameters

An Interpretation spec
analysis. Select the pa
grouped into an experi

Select experiment parameter

☐ Class
☑ Species

Create Interpretation (Step 2 of 4)

Select Profile Plot Display Modes

Select a display mode (Numerical/Categorical) for each parameter.
This information is used only for the Profile Plot View.
For a "Numerical" parameter, each parameter value is connected to the next.
For a "Categorical" parameter, distinct parameter values are not connected.

	Numerical	Categorical
Species	○	●

Create Interpretation (Step 3 of 4)

Select conditions

Select the conditions defined by the selected parameter(s) to include in the interpretation. Samples within a condition are considered as replicates. If Averaged, for each entity, the average intensity value across replicates will be used for visualization and analysis. For experiments with flags, only measurements with permitted flags will be used for visualization and analysis.

Unselect conditions to exclude

☐ [CTRL]
☑ [J0]
☑ [J1]
☑ [J4]
☐ [J5]
☐ [J6]
☐ [J8]
☐ [Jmax10-11]
☐ [Meoh]
☐ [Stds]

■ Select all

Average over replicates in conditions

○ Averaged
○ Non-Averaged
● Both

Use Measurements flagged

☑ Present
☐ Marginal
☐ Absent

Create Interpretation (Step 4 of 4)

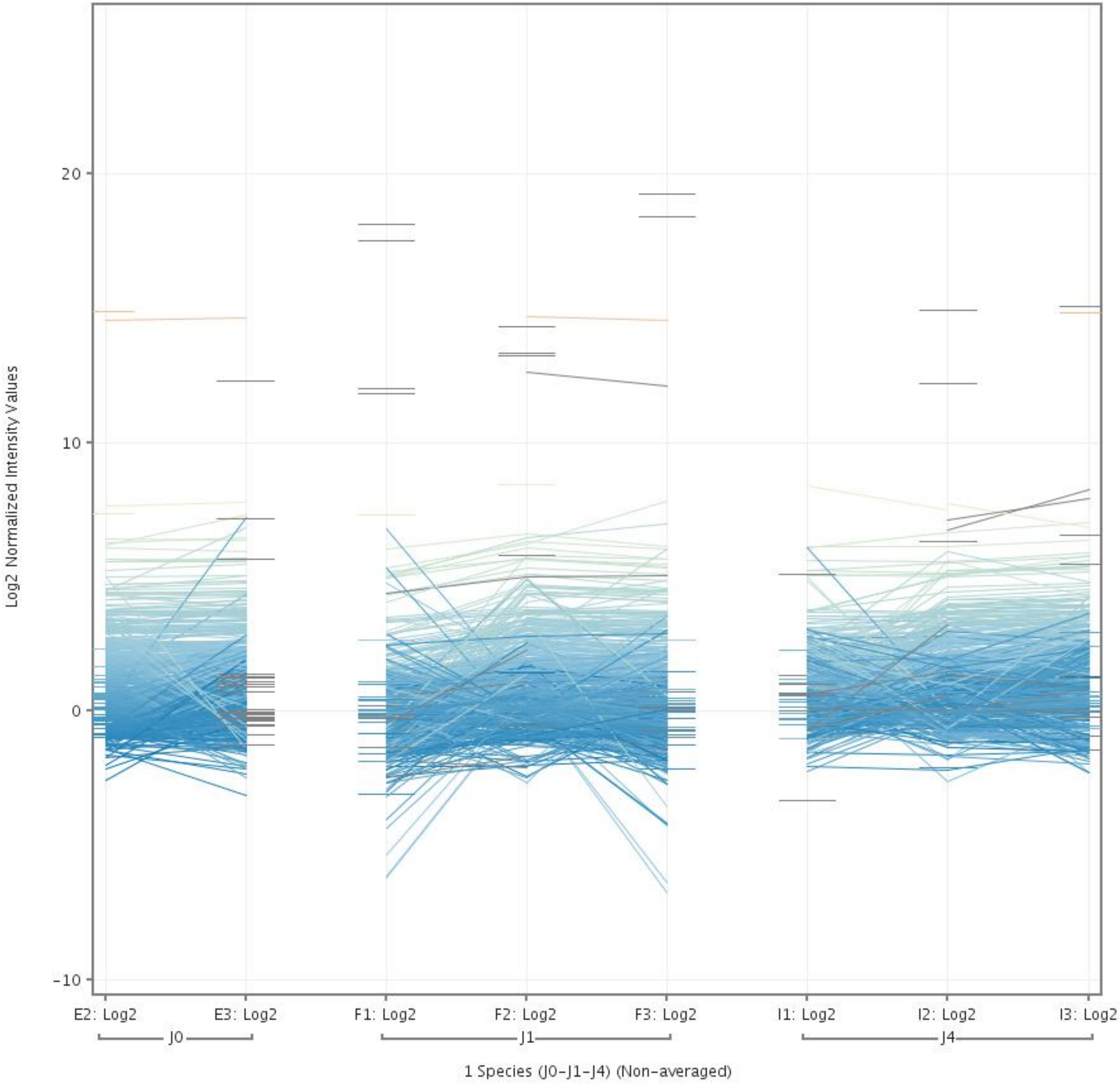
Save Interpretation

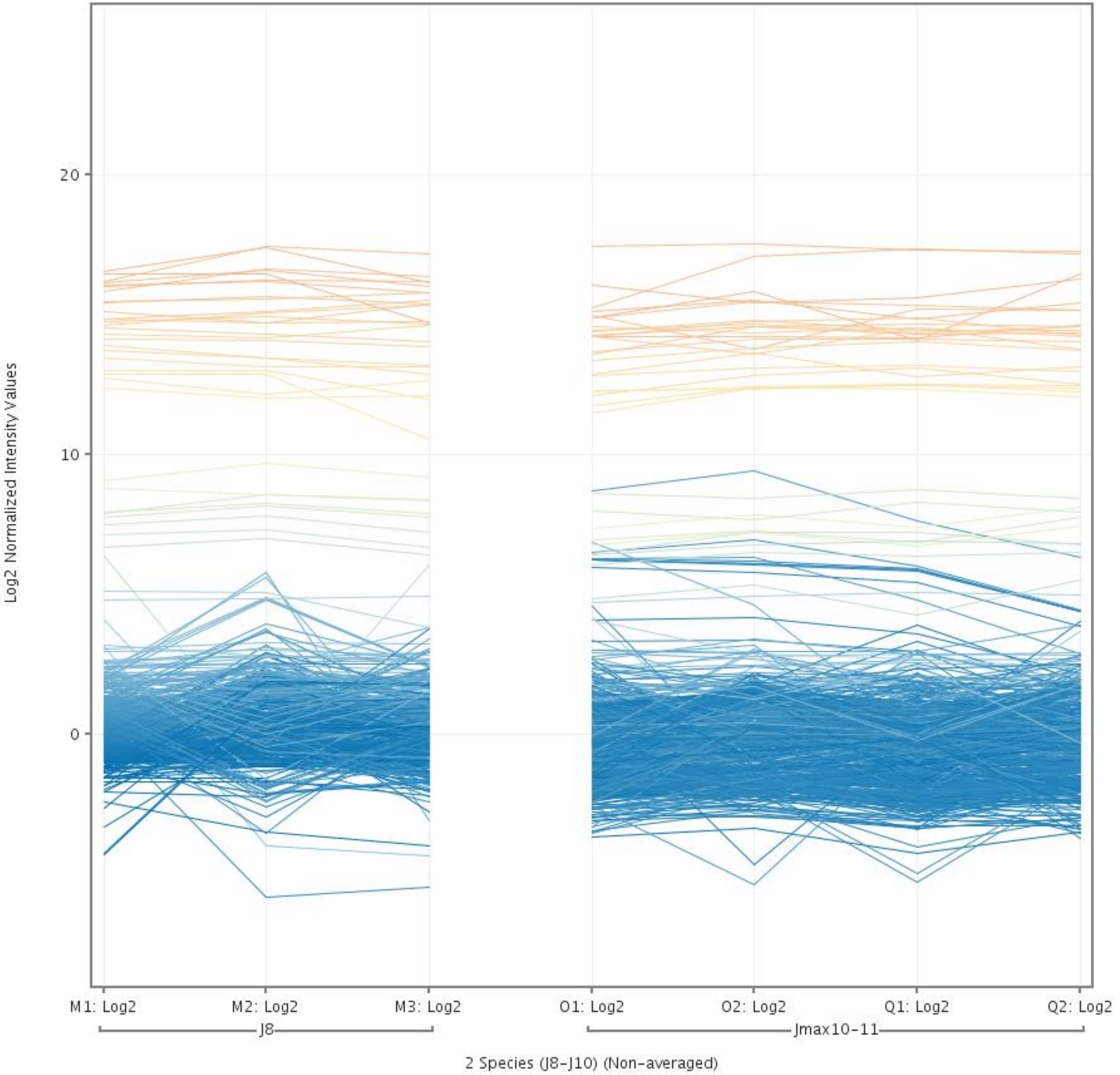
This page displays the details of the interpretation created.

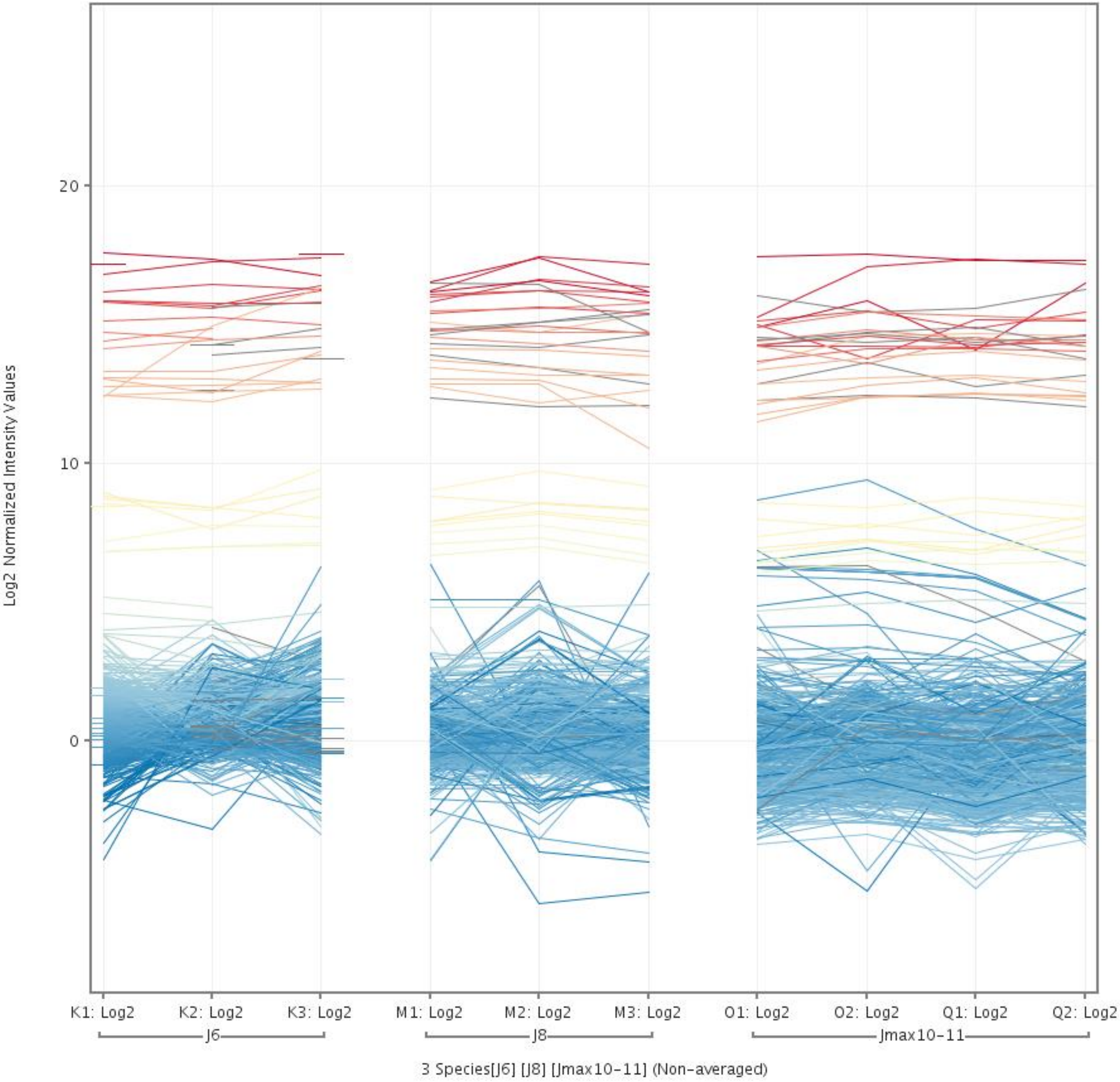
Objects
Species
Species (Non-averag

Name: 1 Species (J0-J1-J4) (Non-averaged)
Notes:
Creation date: Thu Nov 19 15:46:35 CET 2020
Last modified date: Thu Nov 19 15:46:35 CET 2020
Owner: gxuser
Average over replicates in conditions: No

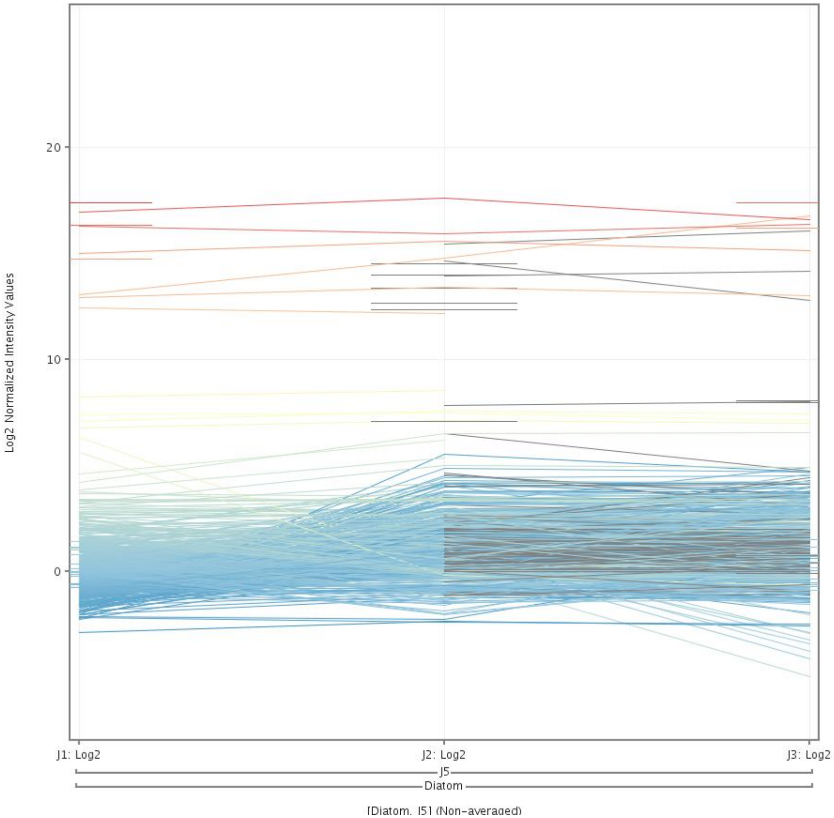
Conditions
[J0]
[J1]
[J4]

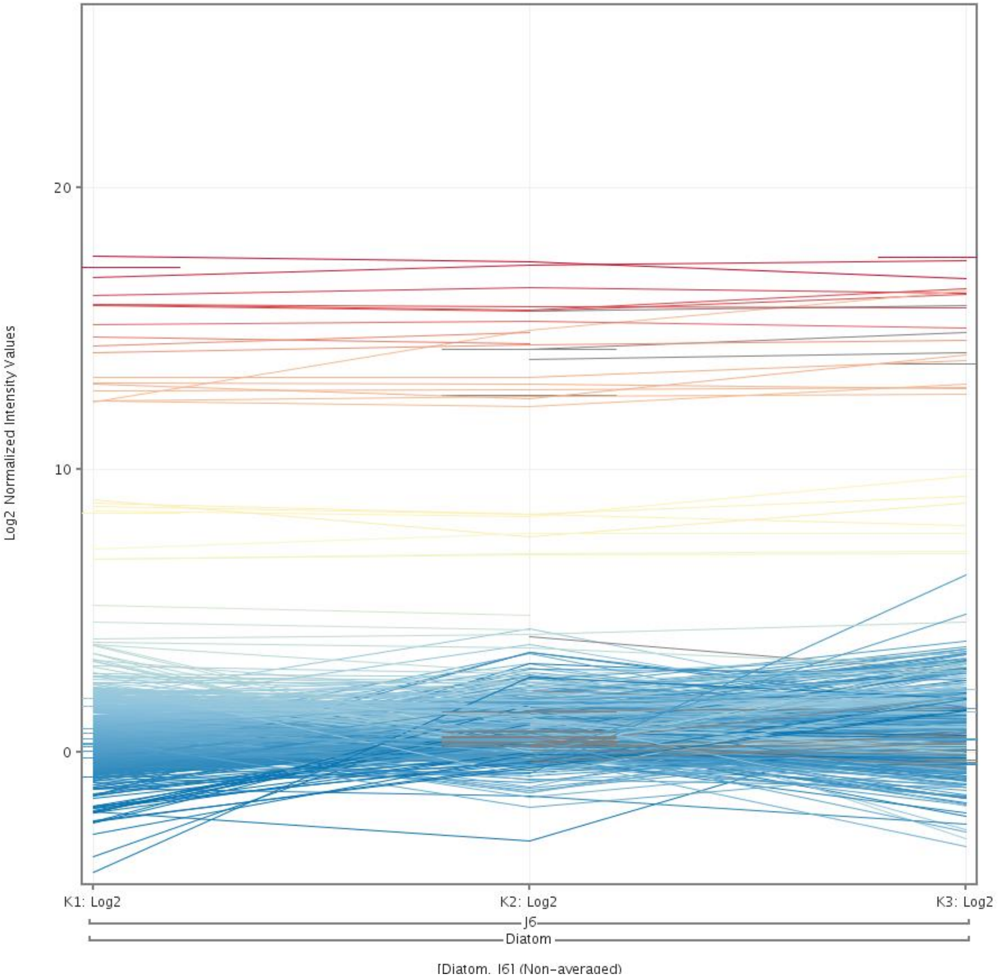

Log2 Normalized Intensity Values
20
10
0
-10
E2: Log2
E3: Log2
F1: Log2
F2: Log2
F3: Log2
I1: Log2
I2: Log2
I3: Log2
J0
J1
J4
1 Species (J0-J1-J4) (Non-averaged)

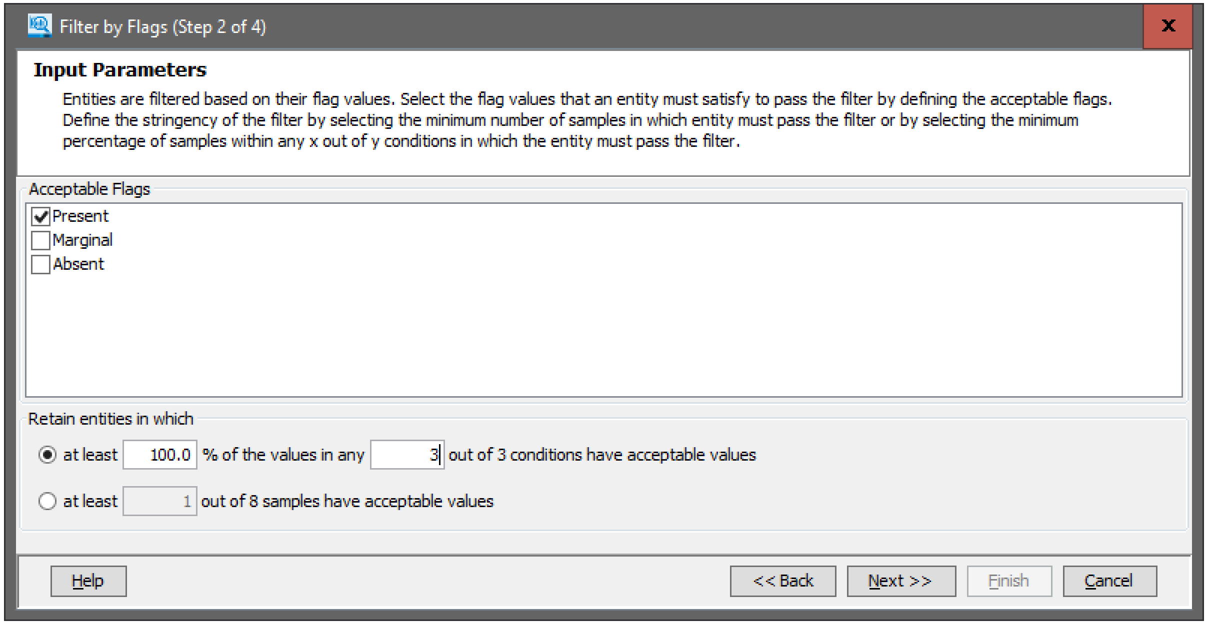

Log2 Normalized Intensity Values
20
10
0
M1: Log2
M2: Log2
M3: Log2
O1: Log2
O2: Log2
Q1: Log2
Q2: Log2
J8
Jmax10-11
2 Species (J8-J10) (Non-averaged)



Log2 Normalized Intensity Values
20
10
0
K1: Log2
K2: Log2
K3: Log2
M1: Log2
M2: Log2
M3: Log2
O1: Log2
O2: Log2
Q1: Log2
Q2: Log2
J6
J8
Jmax10-11
3 Species[J6] [J8] [Jmax10-11] (Non-averaged)


Log2 Normalized Intensity Values
20
10
0
J1: Log2
J2: Log2
J3: Log2
J5
Diatom
[Diatom, J5] (Non-averaged)


Log2 Normalized Intensity Values
20
10
0
K1: Log2
K2: Log2
K3: Log2
J6
Diatom
[Diatom, J6] (Non-averaged)


Filter by Flags (Step 2 of 4)

Input Parameters

Entities are filtered based on their flag values. Select the flag values that an entity must satisfy to pass the filter by defining the acceptable flags. Define the stringency of the filter by selecting the minimum number of samples in which entity must pass the filter or by selecting the minimum percentage of samples within any x out of y conditions in which the entity must pass the filter.

Acceptable Flags

☑ Present
☐ Marginal
☐ Absent

Retain entities in which

● at least 100.0 % of the values in any 3 out of 3 conditions have acceptable values
○ at least 1 out of 8 samples have acceptable values

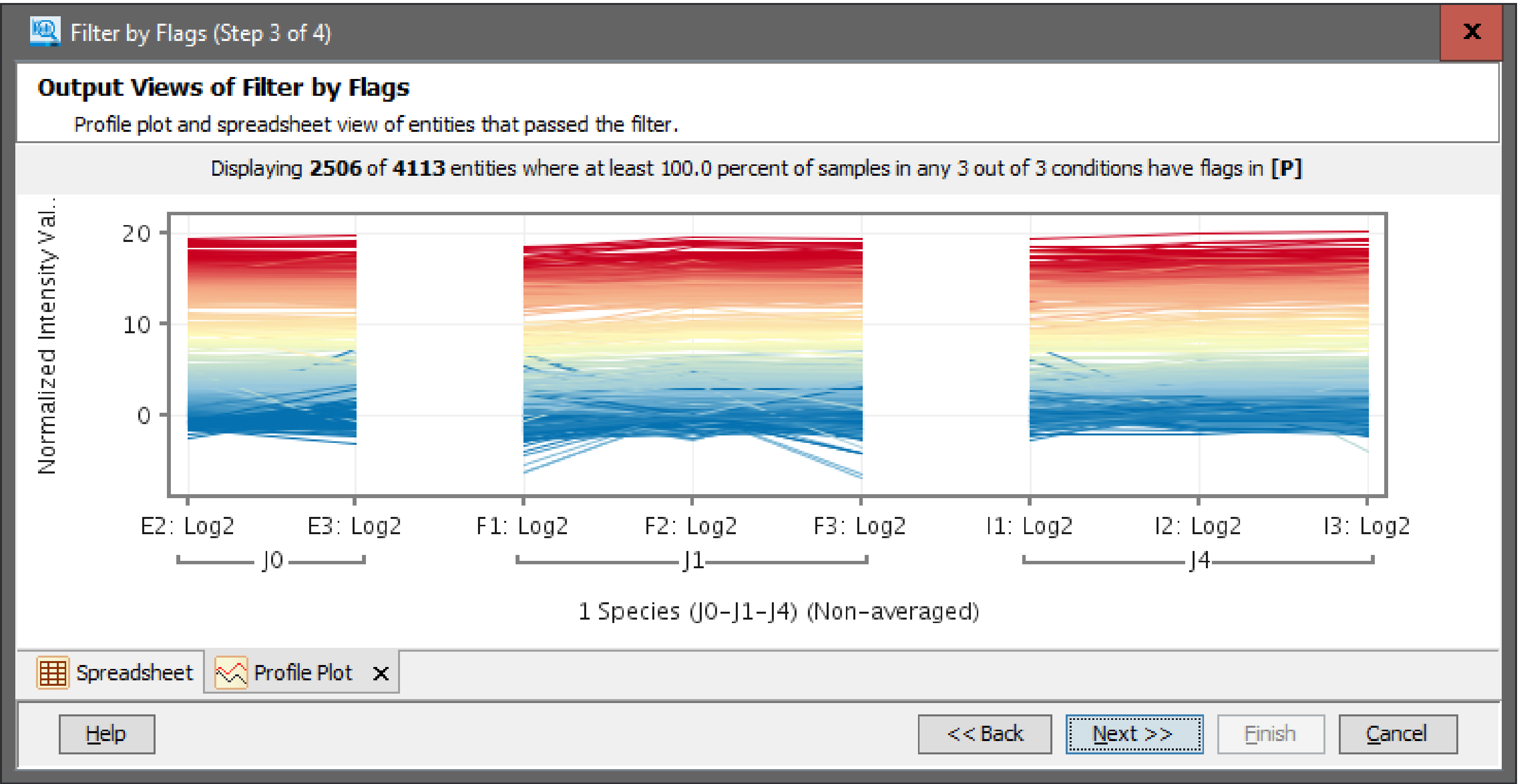
Création de l'analyse I correspondante

Hy1= J0+JJ+J4
- J5
- J6

Hy2= J8+Jmax

Avec hy1 100% of the values in any 3 out of 3 conditions have acceptable values

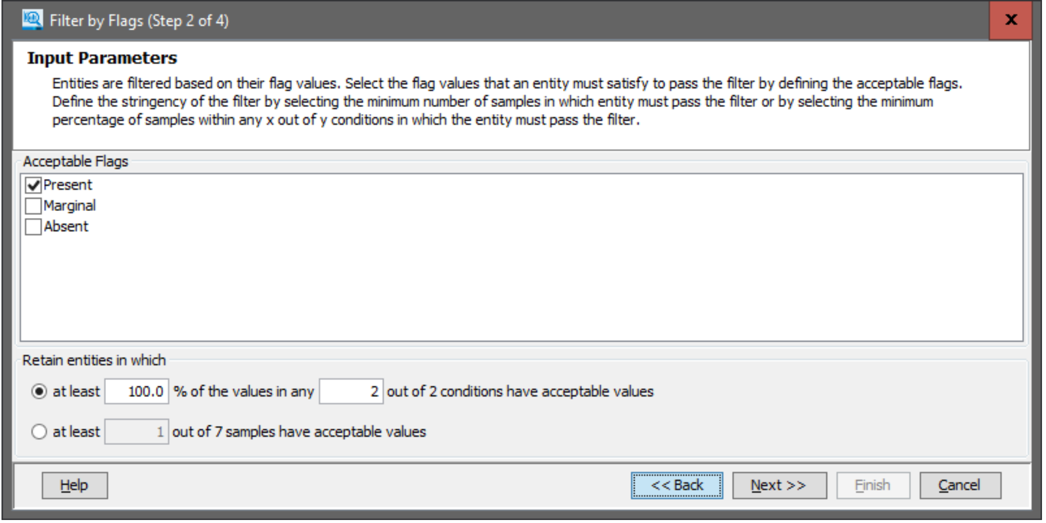
Et Hy2 2 out of 2


Filter by Flags (Step 3 of 4)

Output Views of Filter by Flags

Profile plot and spreadsheet view of entities that passed the filter.

Displaying **2506** of **4113** entities where at least 100.0 percent of samples in any 3 out of 3 conditions have flags in **[P]**



Input Parameters

Entities are filtered based on their flag values. Select the flag values that an entity must satisfy to pass the filter by defining the acceptable flags. Define the stringency of the filter by selecting the minimum number of samples in which entity must pass the filter or by selecting the minimum percentage of samples within any x out of y conditions in which the entity must pass the filter.

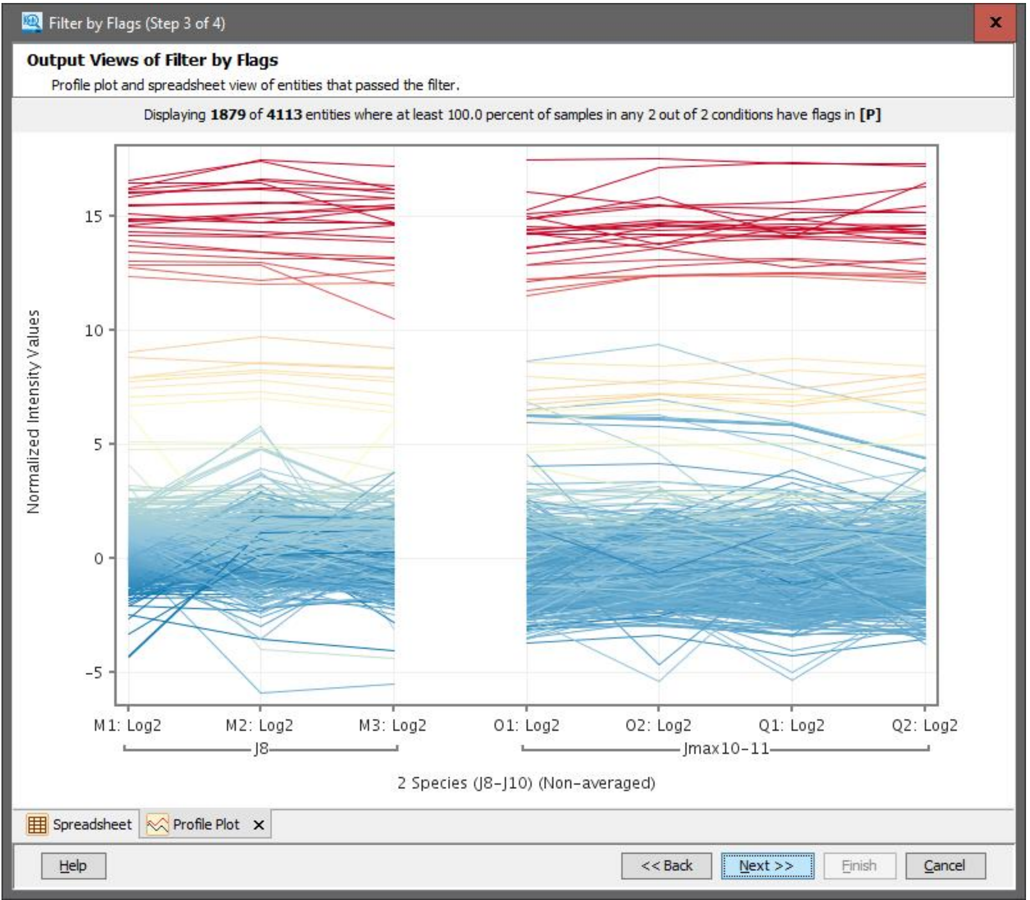
Acceptable Flags

☑ Present
☐ Marginal
☐ Absent

Retain entities in which

● at least 100.0 % of the values in any 2 out of 2 conditions have acceptable values

○ at least 1 out of 7 samples have acceptable values

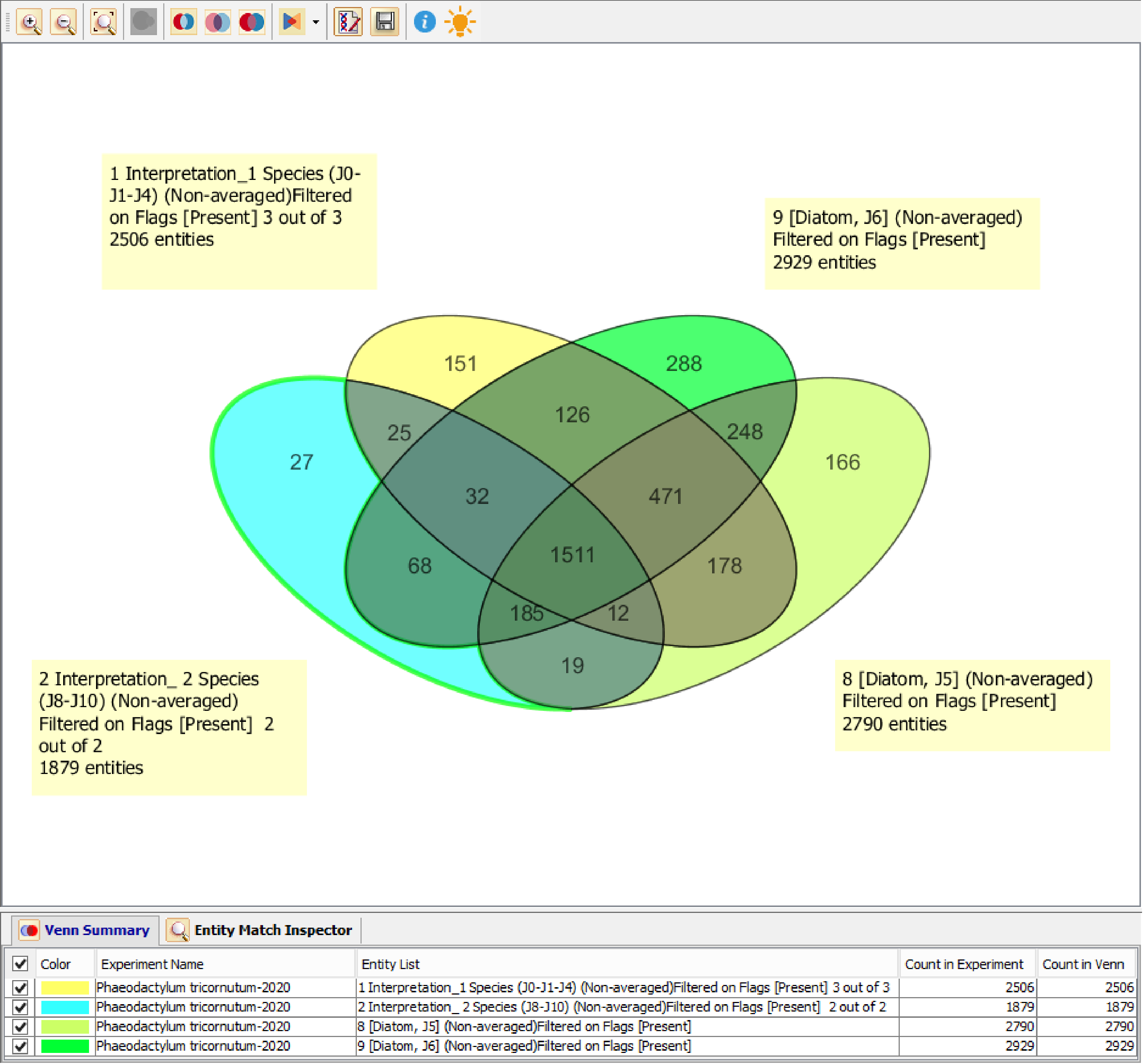


Output Views of Filter by Flags

Profile plot and spreadsheet view of entities that passed the filter.

Displaying **1879** of **4113** entities where at least 100.0 percent of samples in any 2 out of 2 conditions have flags in **[P]**

Et Hy2 2 out of 2



☑	Color	Experiment Name	Entity List	Count in Experiment	Count in Venn
☑	🟨	Phaeodactylum tricornutum-2020	1 Interpretation_1 Species (J0-J1-J4) (Non-averaged)Filtered on Flags [Present] 3 out of 3	2506	2506
☑	🟦	Phaeodactylum tricornutum-2020	2 Interpretation_ 2 Species (J8-J10) (Non-averaged)Filtered on Flags [Present] 2 out of 2	1879	1879
☑	🟩	Phaeodactylum tricornutum-2020	8 [Diatom, J5] (Non-averaged)Filtered on Flags [Present]	2790	2790
☑	🟩	Phaeodactylum tricornutum-2020	9 [Diatom, J6] (Non-averaged)Filtered on Flags [Present]	2929	2929

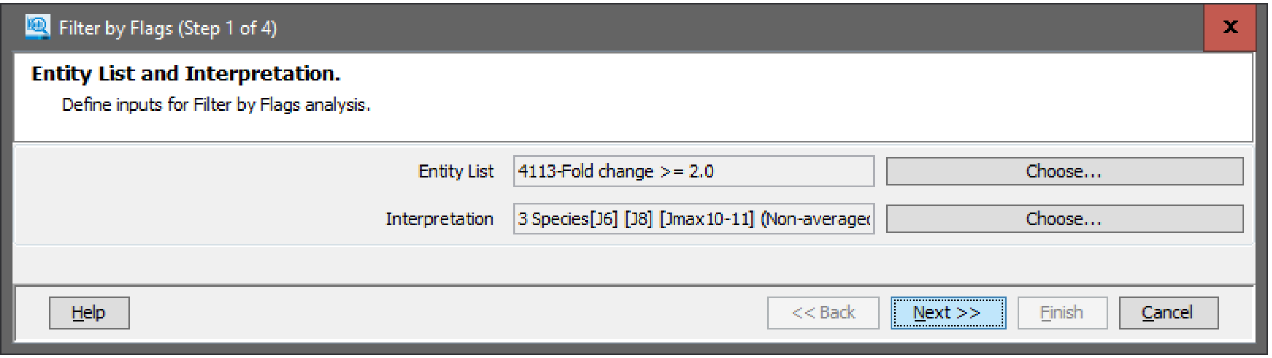
Création de l'analyse II

Hy1= J0+JJ+J4

- J5

- Hy3=J6+ J8+Jmax

Avec hy1 et 3 100% of the values in any 3 out of 3 conditions have acceptable values

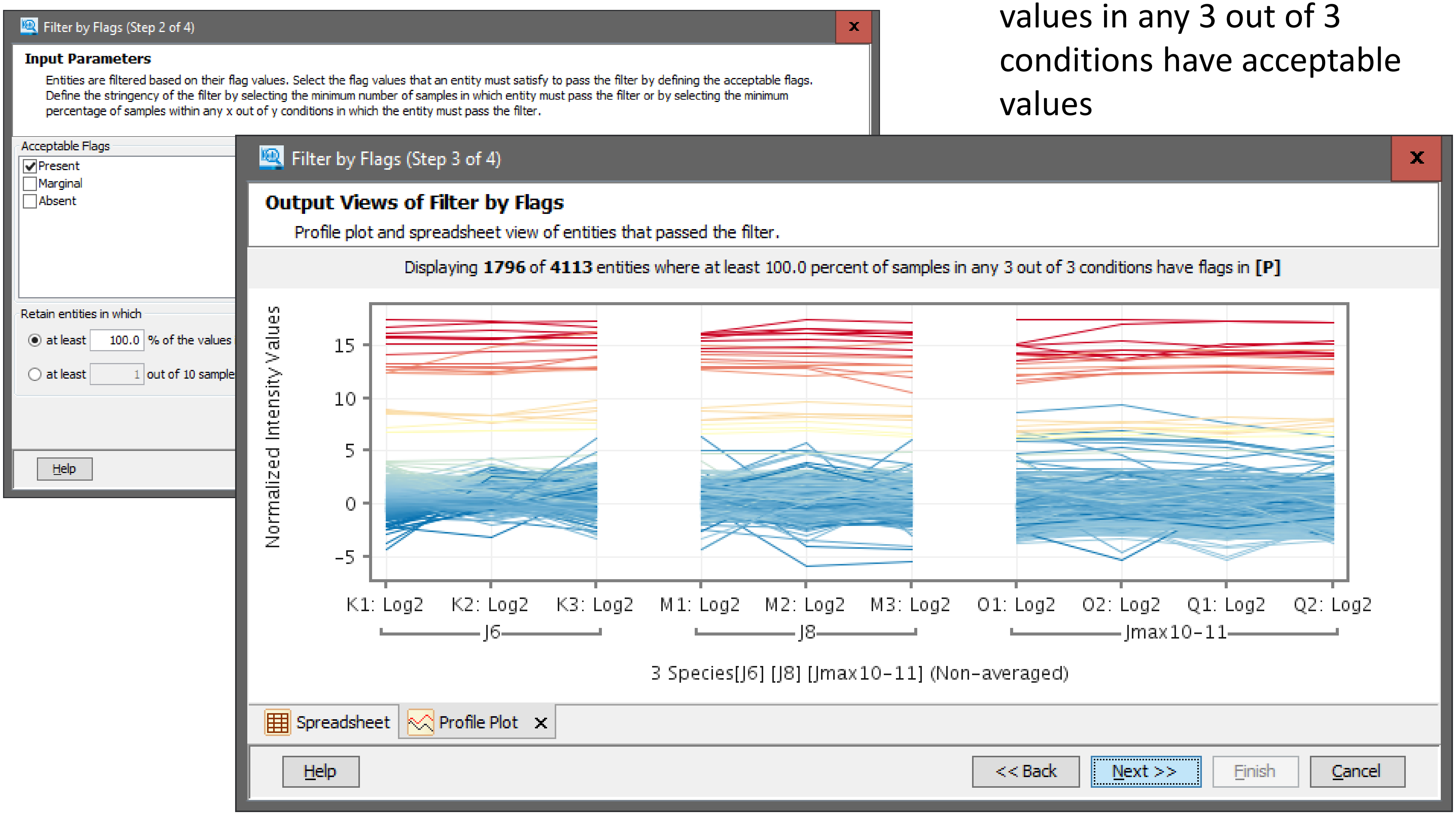


Entity List and Interpretation.

Define inputs for Filter by Flags analysis.

Entity List: 4113-Fold change >= 2.0

Interpretation: 3 Species[J6] [J8] [Jmax10-11] (Non-average



Input Parameters

Entities are filtered based on their flag values. Select the flag values that an entity must satisfy to pass the filter by defining the acceptable flags. Define the stringency of the filter by selecting the minimum number of samples in which entity must pass the filter or by selecting the minimum percentage of samples within any x out of y conditions in which the entity must pass the filter.

Acceptable Flags

☑ Present

☐ Marginal

☐ Absent

Retain entities in which

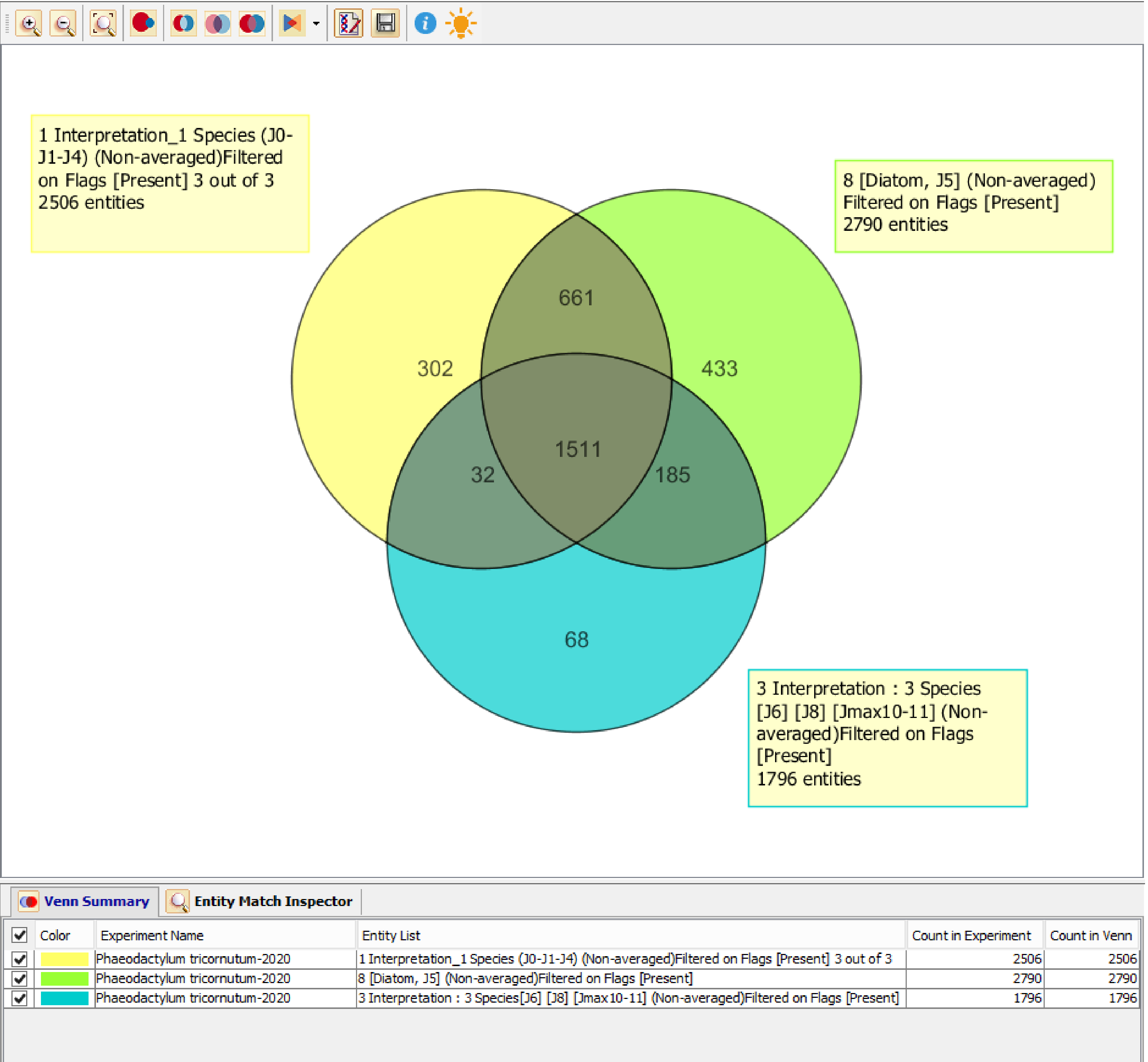
● at least 100.0 % of the values

○ at least 1 out of 10 sample

Output Views of Filter by Flags

Profile plot and spreadsheet view of entities that passed the filter.

Displaying **1796** of **4113** entities where at least 100.0 percent of samples in any 3 out of 3 conditions have flags in **[P]**



☑	Color	Experiment Name	Entity List	Count in Experiment	Count in Venn
☑	🟨	Phaeodactylum tricornutum-2020	1 Interpretation_1 Species (J0-J1-J4) (Non-averaged)Filtered on Flags [Present] 3 out of 3	2506	2506
☑	🟩	Phaeodactylum tricornutum-2020	8 [Diatom, J5] (Non-averaged)Filtered on Flags [Present]	2790	2790
☑	🟦	Phaeodactylum tricornutum-2020	3 Interpretation : 3 Species[J6] [J8] [Jmax10-11] (Non-averaged)Filtered on Flags [Present]	1796	1796

Comparaison

Analyse 1:

Hy1= J0+JJ+J4

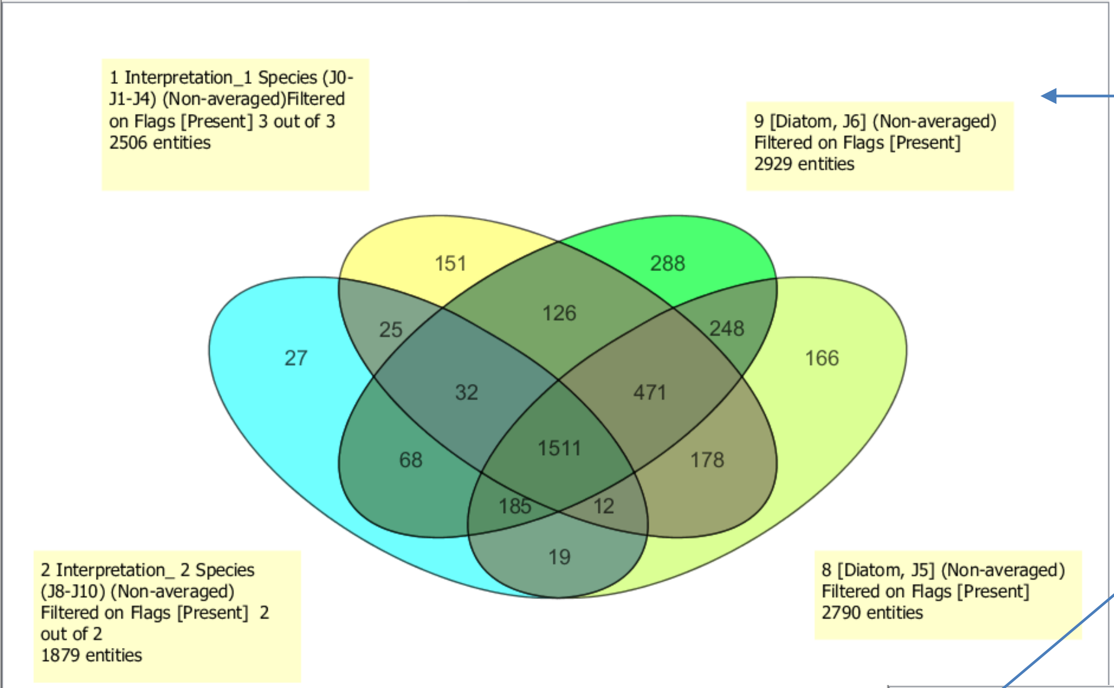
- J5

- J6

Hy2= J8+Jmax

Avec hy1 100% of the values in any 3 out of 3 conditions have acceptable values

Et Hy2 2 out of 2



VS

Analyse II:

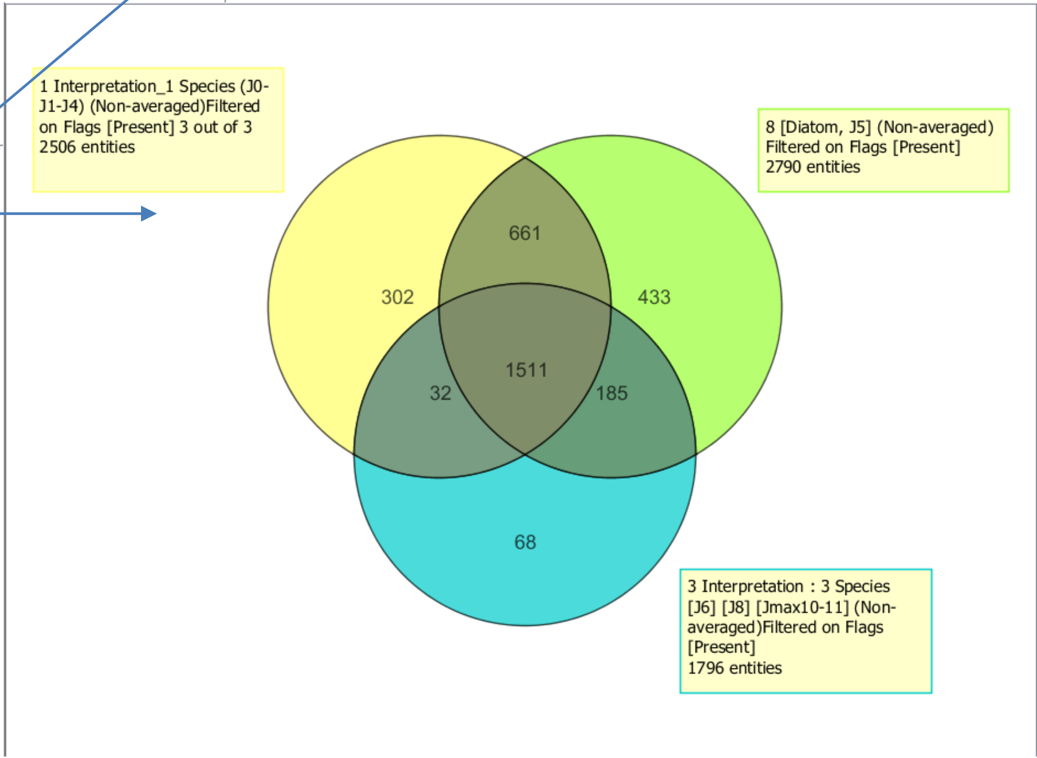
Hy1= J0+JJ+J4

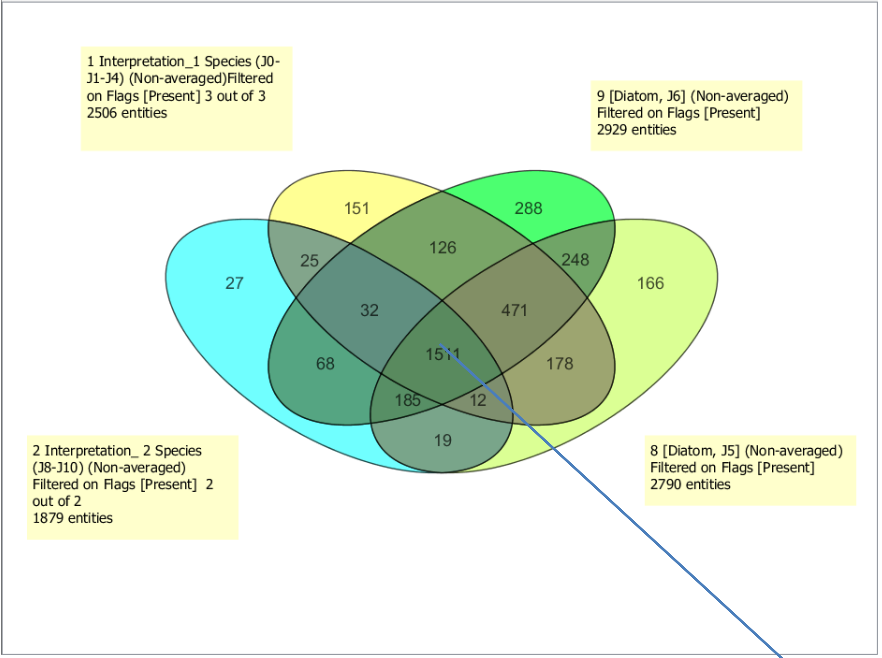
- J5

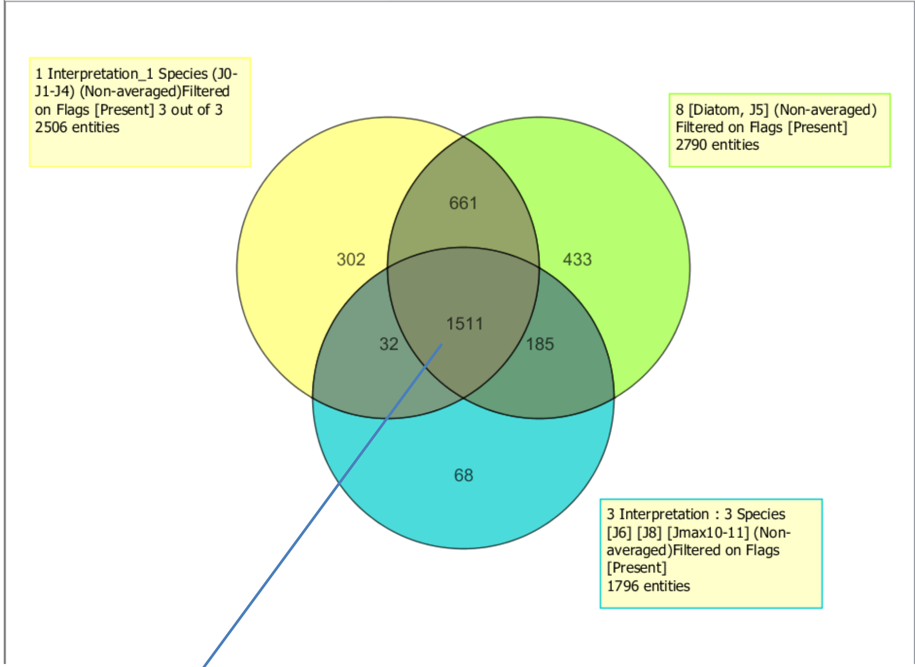
- Hy3=J6+ J8+Jmax

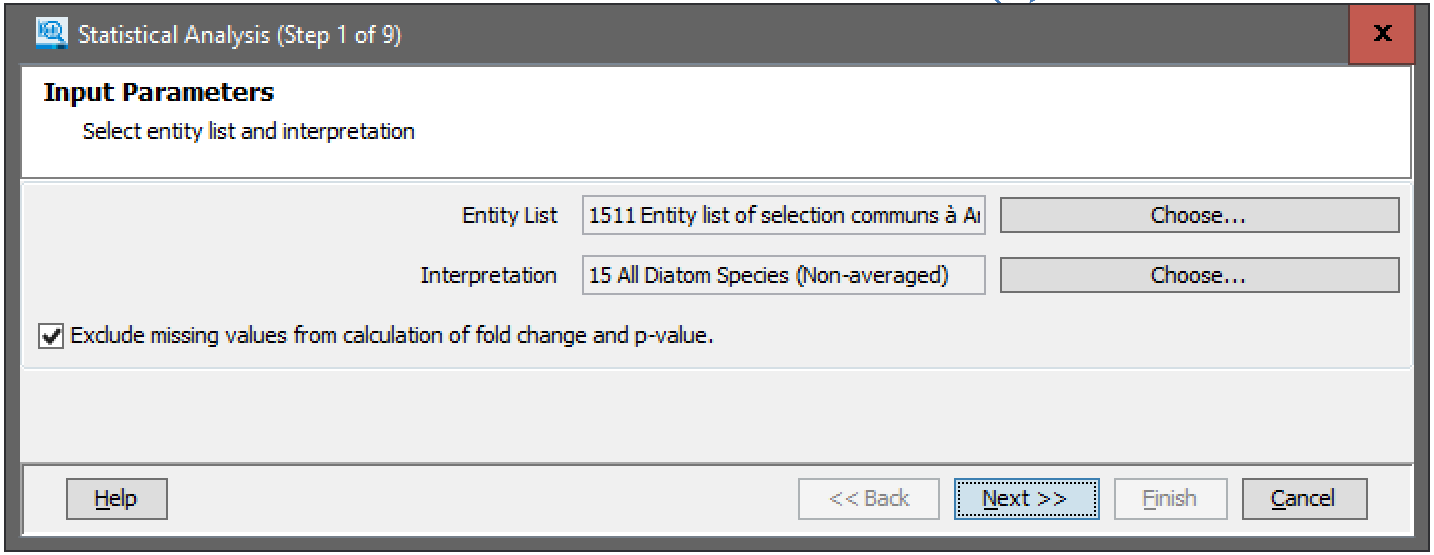
Avec hy1 et Hy3

100% of the values in any 3 out of 3 conditions have acceptable values









Statistical Analysis (Step 1 of 9)

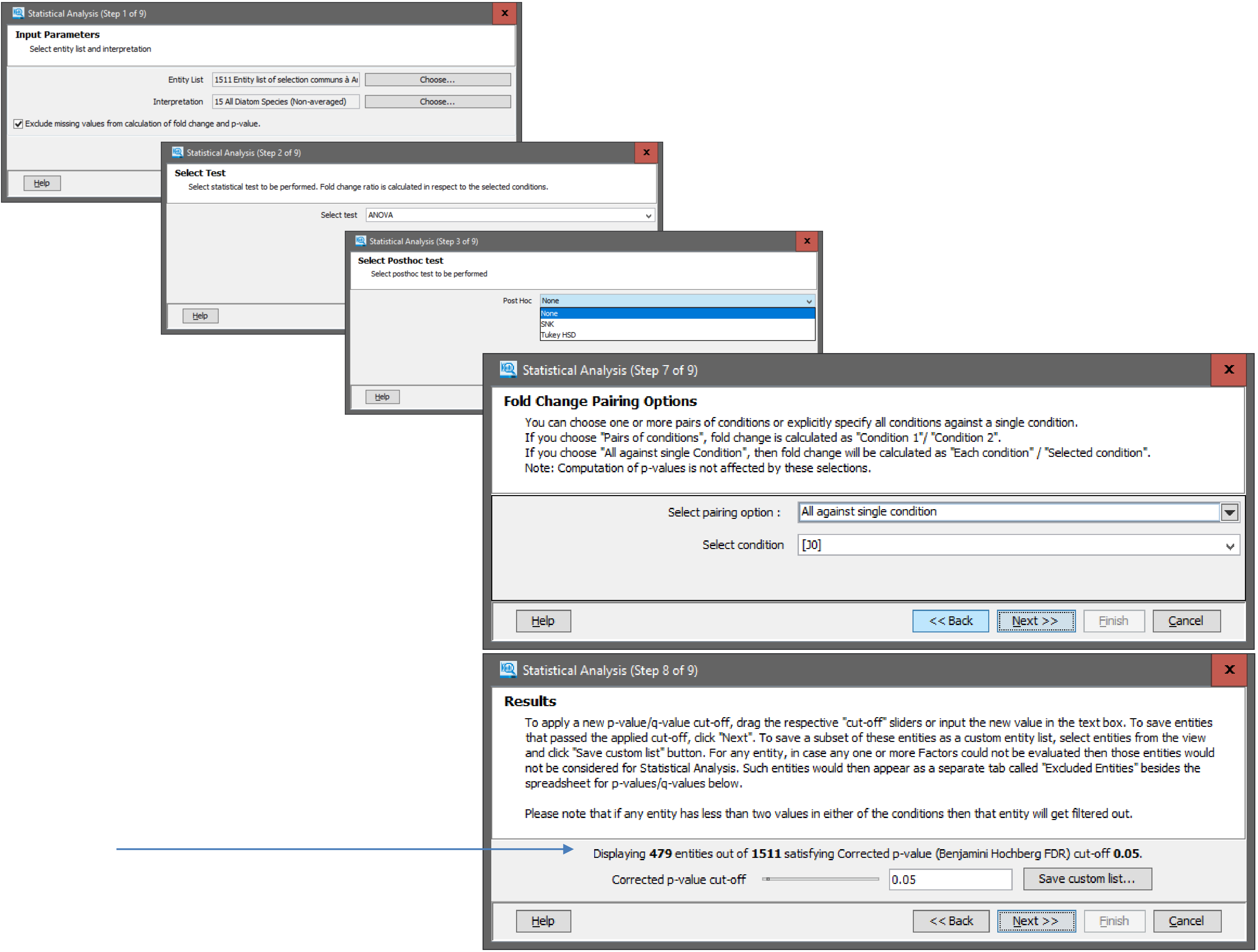
Input Parameters

Select entity list and interpretation

Entity List: 1511 Entity list of selection communs à Ai

Interpretation: 15 All Diatom Species (Non-averaged)

☑ Exclude missing values from calculation of fold change and p-value.



Statistical Analysis (Step 1 of 9)

Input Parameters

Select entity list and interpretation

Entity List: 1511 Entity list of selection communs à A

Interpretation: 15 All Diatom Species (Non-averaged)

☑ Exclude missing values from calculation of fold change and p-value.

Statistical Analysis (Step 2 of 9)

Select Test

Select statistical test to be performed. Fold change ratio is calculated in respect to the selected conditions.

Select test: ANOVA

Statistical Analysis (Step 3 of 9)

Select Posthoc test

Select posthoc test to be performed

Post Hoc: None

Statistical Analysis (Step 7 of 9)

Fold Change Pairing Options

You can choose one or more pairs of conditions or explicitly specify all conditions against a single condition.
If you choose "Pairs of conditions", fold change is calculated as "Condition 1"/ "Condition 2".
If you choose "All against single Condition", then fold change will be calculated as "Each condition" / "Selected condition".
Note: Computation of p-values is not affected by these selections.

Select pairing option : All against single condition

Select condition: [J0]

Statistical Analysis (Step 8 of 9)

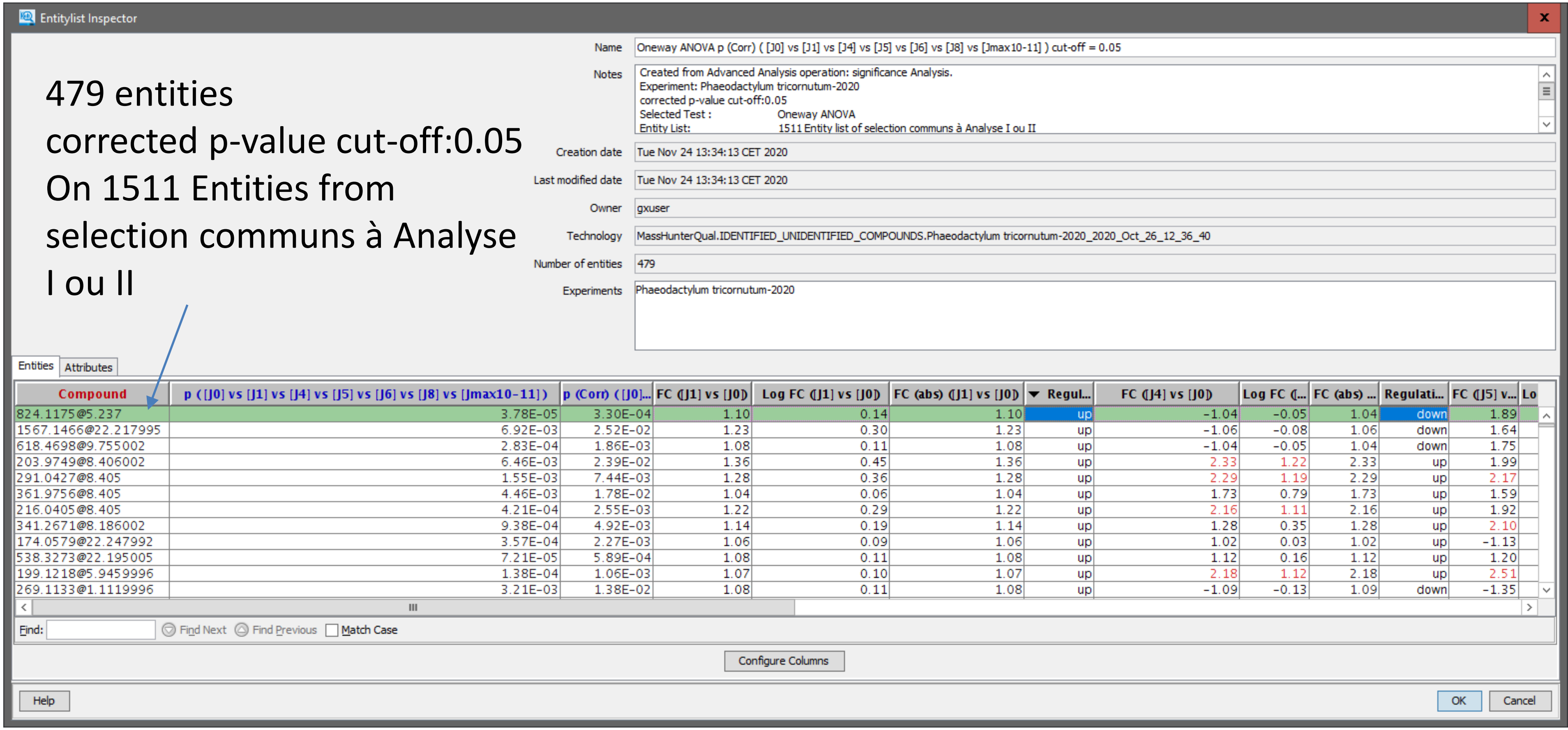
Results

To apply a new p-value/q-value cut-off, drag the respective "cut-off" sliders or input the new value in the text box. To save entities that passed the applied cut-off, click "Next". To save a subset of these entities as a custom entity list, select entities from the view and click "Save custom list" button. For any entity, in case any one or more Factors could not be evaluated then those entities would not be considered for Statistical Analysis. Such entities would then appear as a separate tab called "Excluded Entities" besides the spreadsheet for p-values/q-values below.

Please note that if any entity has less than two values in either of the conditions then that entity will get filtered out.

Displaying **479** entities out of **1511** satisfying Corrected p-value (Benjamini Hochberg FDR) cut-off **0.05**.

Corrected p-value cut-off: 0.05



479 entities
corrected p-value cut-off:0.05
On 1511 Entities from
selection communs à Analyse
I ou II

Name: Oneway ANOVA p (Corr) ([J0] vs [J1] vs [J4] vs [J5] vs [J6] vs [J8] vs [Jmax10-11]) cut-off = 0.05

Notes: Created from Advanced Analysis operation: significance Analysis.
Experiment: Phaeodactylum tricornutum-2020
corrected p-value cut-off:0.05
Selected Test : Oneway ANOVA
Entity List: 1511 Entity list of selection communs à Analyse I ou II

Creation date: Tue Nov 24 13:34:13 CET 2020

Last modified date: Tue Nov 24 13:34:13 CET 2020

Owner: gxuser

Technology: MassHunterQual.IDENTIFIED_UNIDENTIFIED_COMPOUNDS.Phaeodactylum tricornutum-2020_2020_Oct_26_12_36_40

Number of entities: 479

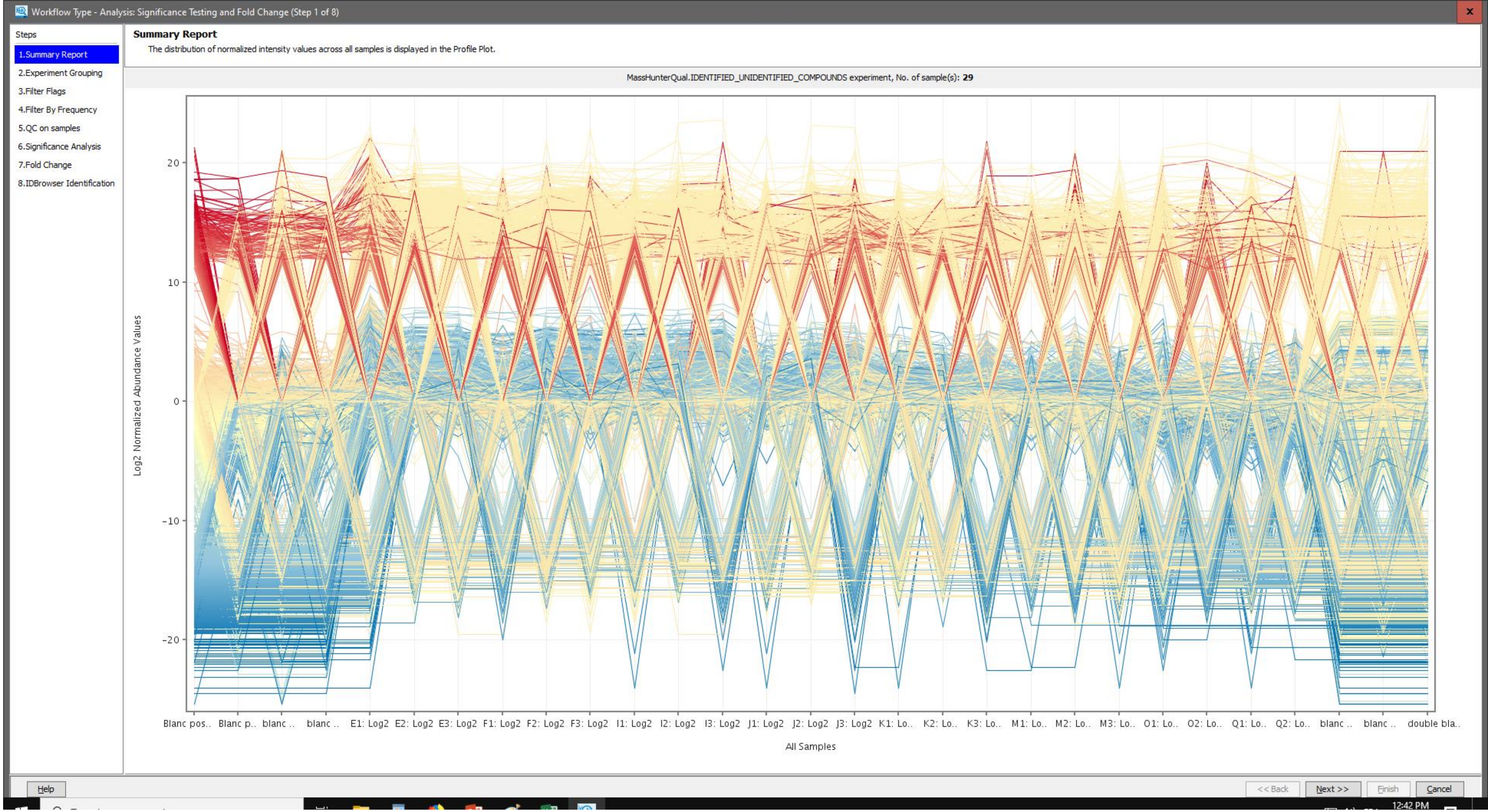
Experiments: Phaeodactylum tricornutum-2020

Compound	p ([J0] vs [J1] vs [J4] vs [J5] vs [J6] vs [J8] vs [Jmax10-11])	p (Corr) ([J0]...	FC ([J1] vs [J0])	Log FC ([J1] vs [J0])	FC (abs) ([J1] vs [J0])	▼ Regul...	FC ([J4] vs [J0])	Log FC ([...	FC (abs) ...	Regulati...	FC ([J5] v...	Lo
824.1175@5.237	3.78E-05	3.30E-04	1.10	0.14	1.10	up	-1.04	-0.05	1.04	down	1.89	
1567.1466@22.217995	6.92E-03	2.52E-02	1.23	0.30	1.23	up	-1.06	-0.08	1.06	down	1.64	
618.4698@9.755002	2.83E-04	1.86E-03	1.08	0.11	1.08	up	-1.04	-0.05	1.04	down	1.75	
203.9749@8.406002	6.46E-03	2.39E-02	1.36	0.45	1.36	up	2.33	1.22	2.33	up	1.99	
291.0427@8.405	1.55E-03	7.44E-03	1.28	0.36	1.28	up	2.29	1.19	2.29	up	2.17	
361.9756@8.405	4.46E-03	1.78E-02	1.04	0.06	1.04	up	1.73	0.79	1.73	up	1.59	
216.0405@8.405	4.21E-04	2.55E-03	1.22	0.29	1.22	up	2.16	1.11	2.16	up	1.92	
341.2671@8.186002	9.38E-04	4.92E-03	1.14	0.19	1.14	up	1.28	0.35	1.28	up	2.10	
174.0579@22.247992	3.57E-04	2.27E-03	1.06	0.09	1.06	up	1.02	0.03	1.02	up	-1.13	
538.3273@22.195005	7.21E-05	5.89E-04	1.08	0.11	1.08	up	1.12	0.16	1.12	up	1.20	
199.1218@5.9459996	1.38E-04	1.06E-03	1.07	0.10	1.07	up	2.18	1.12	2.18	up	2.51	
269.1133@1.1119996	3.21E-03	1.38E-02	1.08	0.11	1.08	up	-1.09	-0.13	1.09	down	-1.35	

Find: ☐ Match Case

Created from Advanced Analysis operation: significance Analysis.
Experiment: Phaeodactylum tricornutum-2020
corrected p-value cut-off:0.05
Selected Test : Oneway ANOVA
Entity List: 1511 Entity list of selection communs à Analyse I ou II
Interpretation: 15 All Diatom Species (Non-averaged)
p-value computation: Asymptotic
Multiple Testing Correction: Benjamini-Hochberg

SUITE II

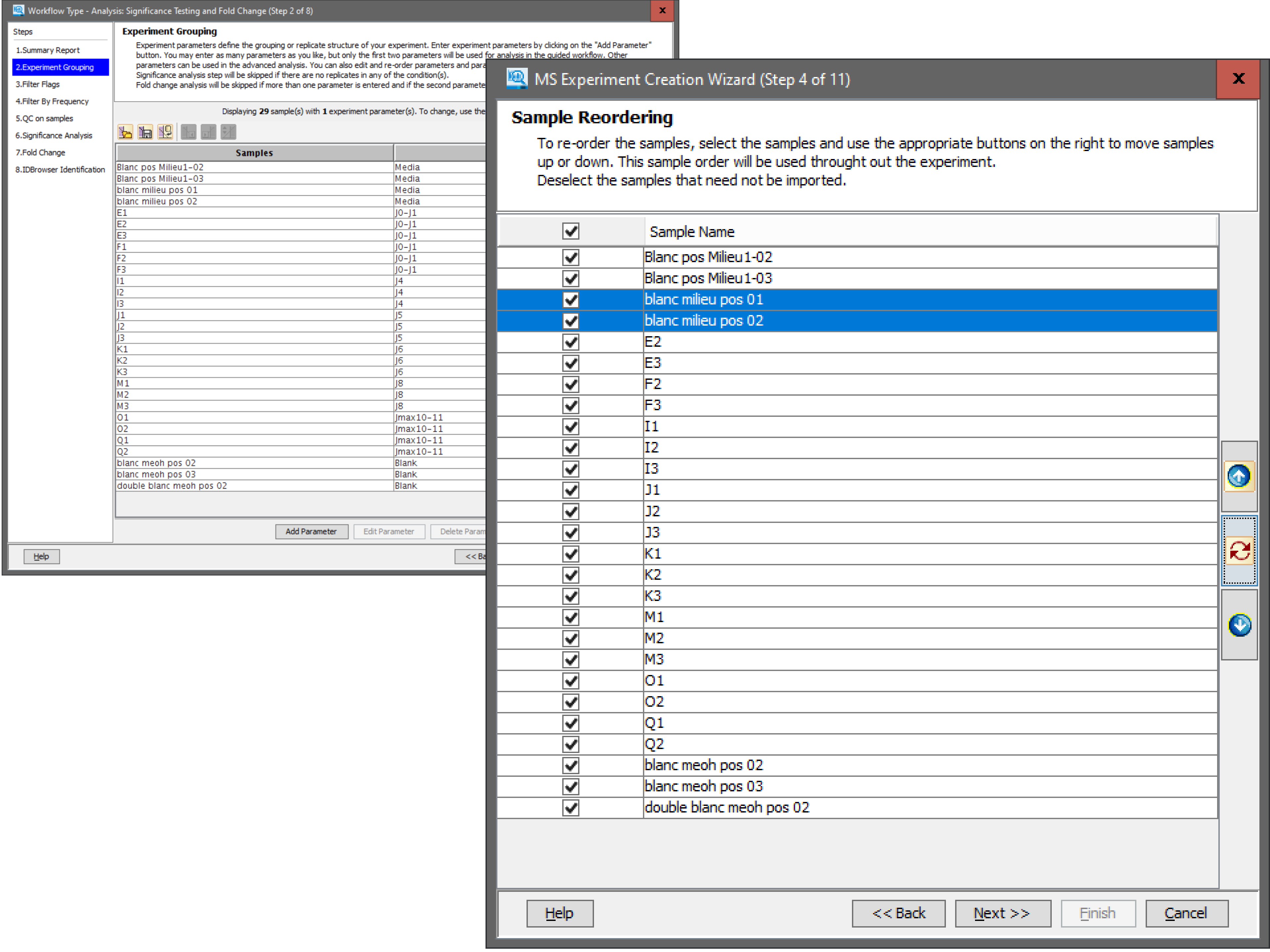


Summary Report

The distribution of normalized intensity values across all samples is displayed in the Profile Plot.

MassHunterQual.IDENTIFIED_UNIDENTIFIED_COMPOUNDS experiment, No. of sample(s): **29**

Nouvel « experiment » basé sur 27 échantillons seulement Phaeodactylum (without E1 et F1)+ Media + Solvant



Experiment Grouping

Experiment parameters define the grouping or replicate structure of your experiment. Enter experiment parameters by clicking on the "Add Parameter" button. You may enter as many parameters as you like, but only the first two parameters will be used for analysis in the guided workflow. Other parameters can be used in the advanced analysis. You can also edit and re-order parameters and para

Significance analysis step will be skipped if there are no replicates in any of the condition(s).

Fold change analysis will be skipped if more than one parameter is entered and if the second paramete

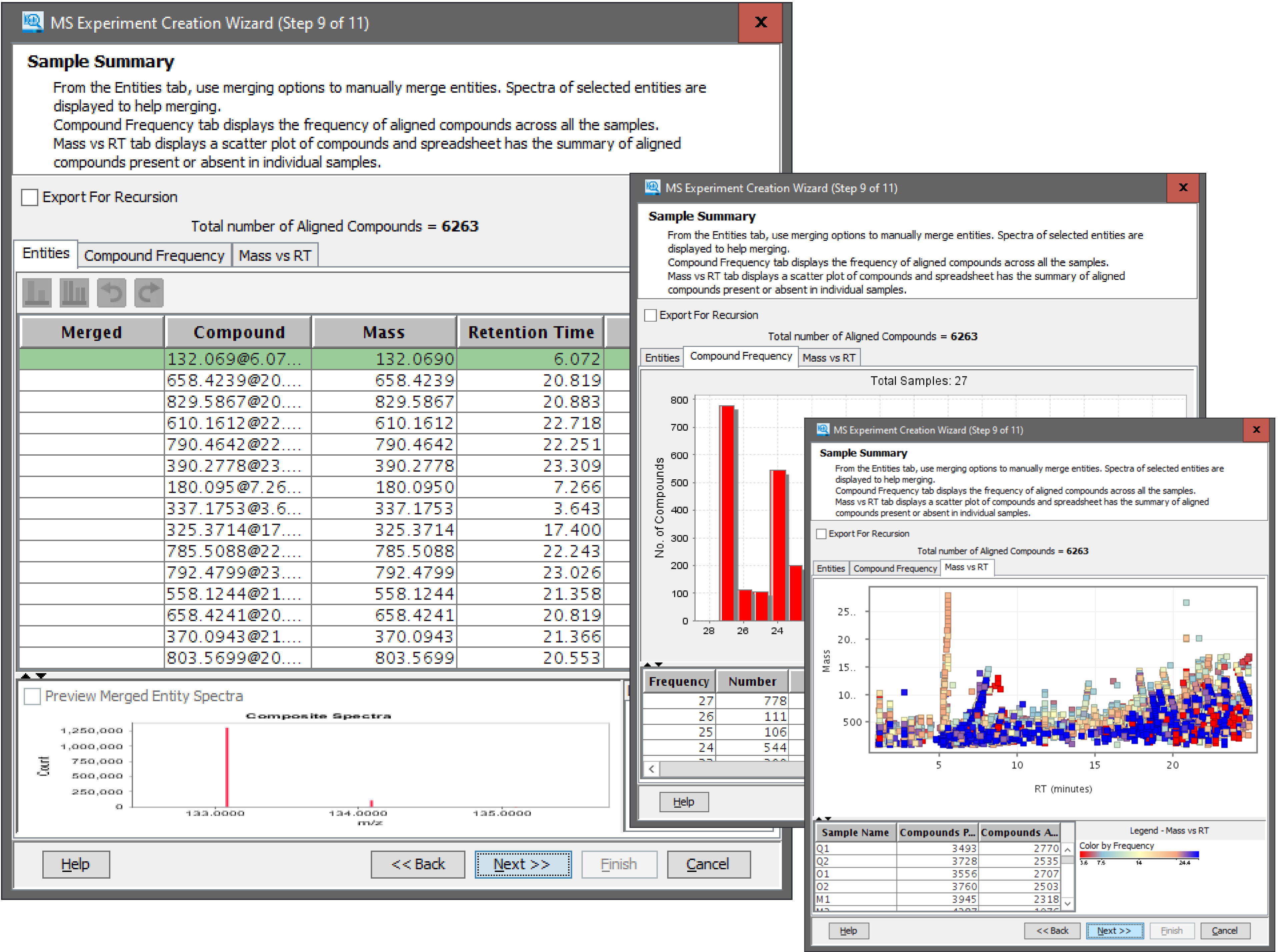
Displaying **29** sample(s) with **1** experiment parameter(s). To change, use the

Samples	
Blanc pos Milieu1-02	Media
Blanc pos Milieu1-03	Media
blanc milieu pos 01	Media
blanc milieu pos 02	Media
E1	J0-J1
E2	J0-J1
E3	J0-J1
F1	J0-J1
F2	J0-J1
F3	J0-J1
I1	J4
I2	J4
I3	J4
J1	J5
J2	J5
J3	J5
K1	J6
K2	J6
K3	J6
M1	J8
M2	J8
M3	J8
O1	Jmax10-11
O2	Jmax10-11
Q1	Jmax10-11
Q2	Jmax10-11
blanc meoh pos 02	Blank
blanc meoh pos 03	Blank
double blanc meoh pos 02	Blank

Sample Reordering

To re-order the samples, select the samples and use the appropriate buttons on the right to move samples up or down. This sample order will be used throught out the experiment.
Deselect the samples that need not be imported.

☑	Sample Name
☑	Blanc pos Milieu1-02
☑	Blanc pos Milieu1-03
☑	blanc milieu pos 01
☑	blanc milieu pos 02
☑	E2
☑	E3
☑	F2
☑	F3
☑	I1
☑	I2
☑	I3
☑	J1
☑	J2
☑	J3
☑	K1
☑	K2
☑	K3
☑	M1
☑	M2
☑	M3
☑	O1
☑	O2
☑	Q1
☑	Q2
☑	blanc meoh pos 02
☑	blanc meoh pos 03
☑	double blanc meoh pos 02



MS Experiment Creation Wizard (Step 9 of 11)

Sample Summary

From the Entities tab, use merging options to manually merge entities. Spectra of selected entities are displayed to help merging.
Compound Frequency tab displays the frequency of aligned compounds across all the samples.
Mass vs RT tab displays a scatter plot of compounds and spreadsheet has the summary of aligned compounds present or absent in individual samples.

☐ Export For Recursion

Total number of Aligned Compounds = **6263**

Merged	Compound	Mass	Retention Time
	132.069@6.07...	132.0690	6.072
	658.4239@20....	658.4239	20.819
	829.5867@20....	829.5867	20.883
	610.1612@22....	610.1612	22.718
	790.4642@22....	790.4642	22.251
	390.2778@23....	390.2778	23.309
	180.095@7.26...	180.0950	7.266
	337.1753@3.6...	337.1753	3.643
	325.3714@17....	325.3714	17.400
	785.5088@22....	785.5088	22.243
	792.4799@23....	792.4799	23.026
	558.1244@21....	558.1244	21.358
	658.4241@20....	658.4241	20.819
	370.0943@21....	370.0943	21.366
	803.5699@20....	803.5699	20.553

☐ Preview Merged Entity Spectra

MS Experiment Creation Wizard (Step 9 of 11)

Sample Summary

From the Entities tab, use merging options to manually merge entities. Spectra of selected entities are displayed to help merging.
Compound Frequency tab displays the frequency of aligned compounds across all the samples.
Mass vs RT tab displays a scatter plot of compounds and spreadsheet has the summary of aligned compounds present or absent in individual samples.

☐ Export For Recursion

Total number of Aligned Compounds = **6263**

Frequency	Number
27	778
26	111
25	106
24	544

MS Experiment Creation Wizard (Step 9 of 11)

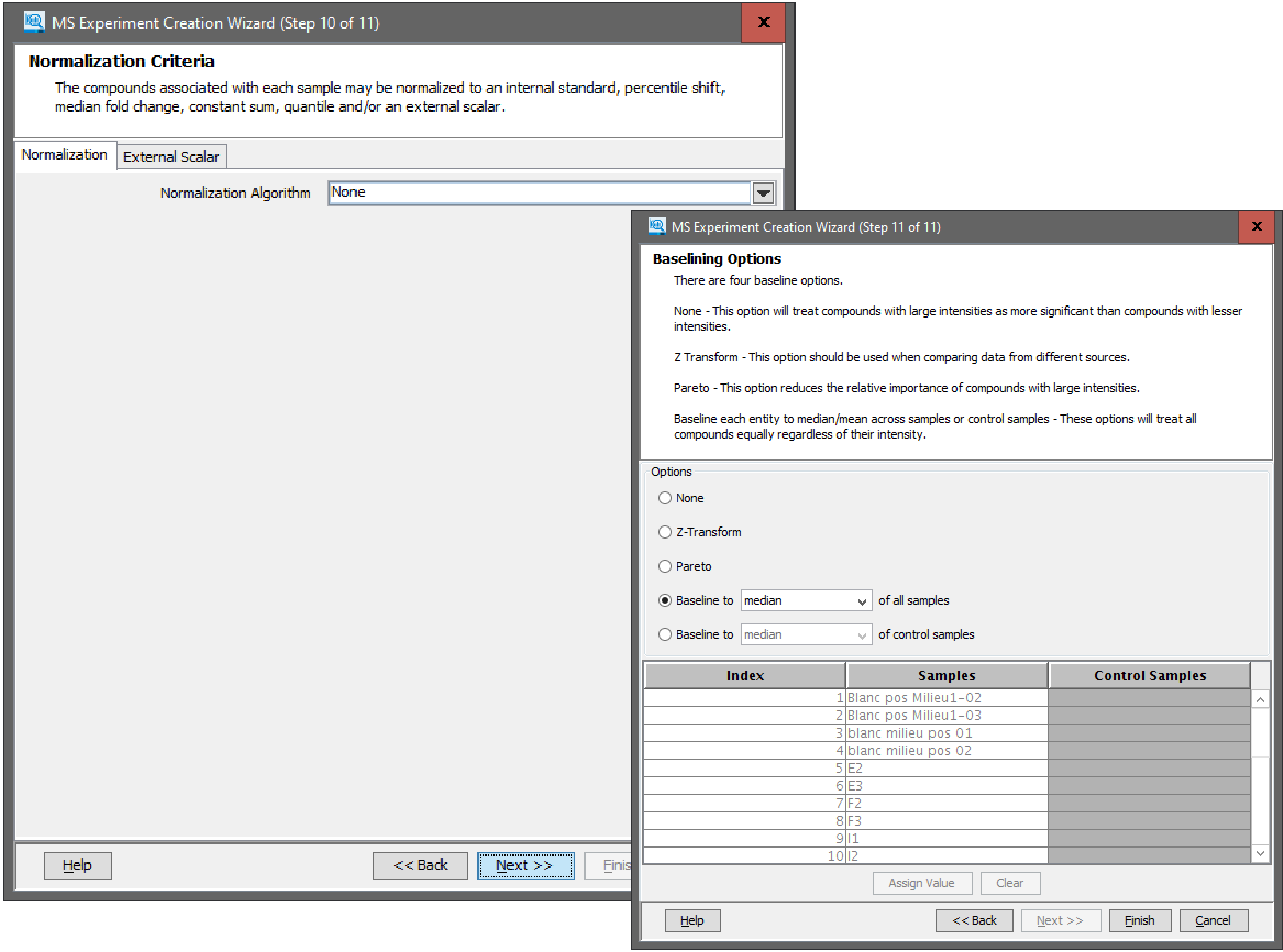
Sample Summary

From the Entities tab, use merging options to manually merge entities. Spectra of selected entities are displayed to help merging.
Compound Frequency tab displays the frequency of aligned compounds across all the samples.
Mass vs RT tab displays a scatter plot of compounds and spreadsheet has the summary of aligned compounds present or absent in individual samples.

☐ Export For Recursion

Total number of Aligned Compounds = **6263**

Sample Name	Compounds P...	Compounds A...
Q1	3493	2770
Q2	3728	2535
O1	3556	2707
O2	3760	2503
M1	3945	2318



MS Experiment Creation Wizard (Step 10 of 11)

Normalization Criteria

The compounds associated with each sample may be normalized to an internal standard, percentile shift, median fold change, constant sum, quantile and/or an external scalar.

Normalization Algorithm: None

MS Experiment Creation Wizard (Step 11 of 11)

Baselining Options

There are four baseline options.

None - This option will treat compounds with large intensities as more significant than compounds with lesser intensities.

Z Transform - This option should be used when comparing data from different sources.

Pareto - This option reduces the relative importance of compounds with large intensities.

Baseline each entity to median/mean across samples or control samples - These options will treat all compounds equally regardless of their intensity.

Options

○ None

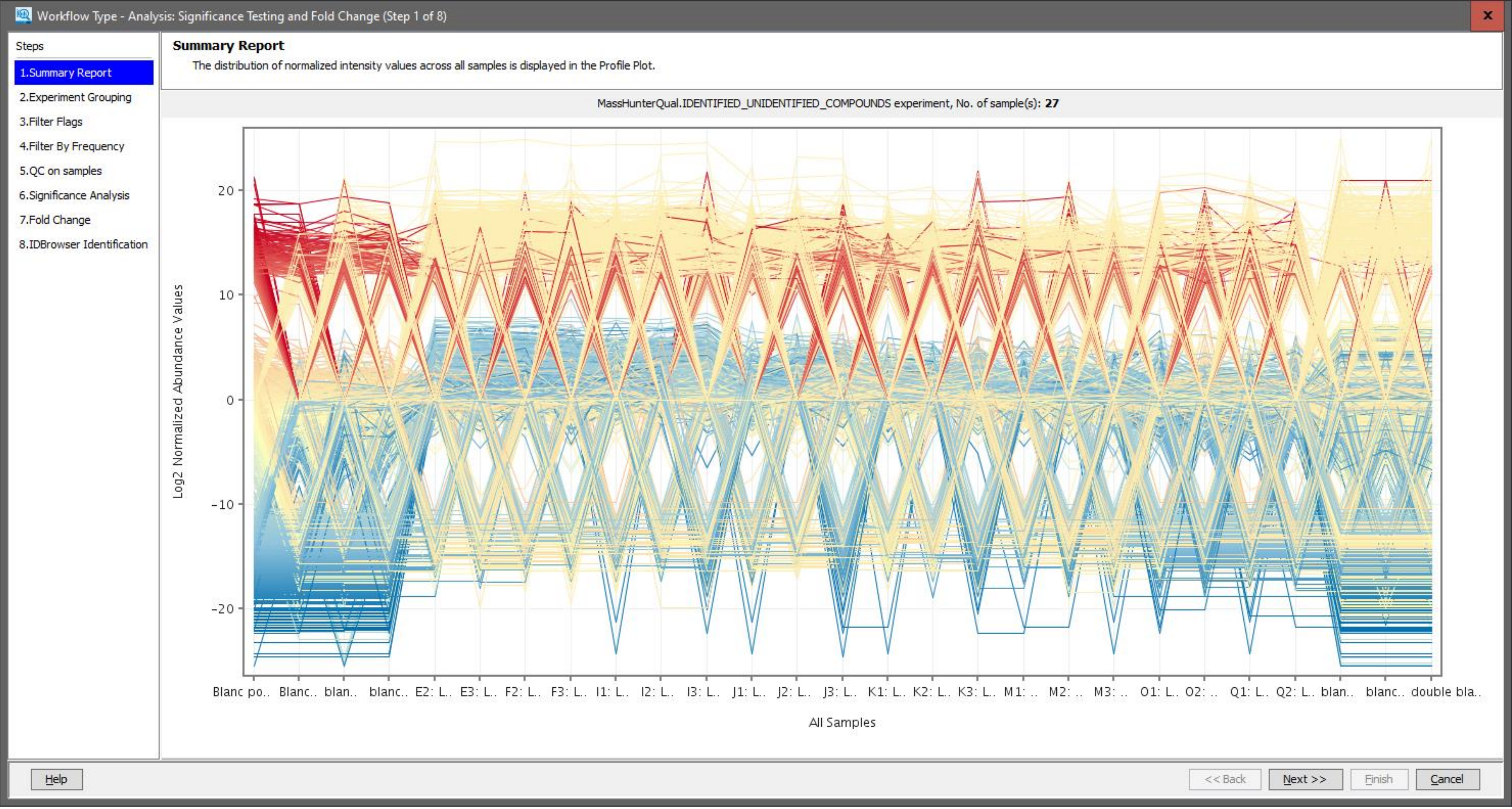
○ Z-Transform

○ Pareto

● Baseline to median of all samples

○ Baseline to median of control samples

Index	Samples	Control Samples
1	Blanc pos Milieu1-02	
2	Blanc pos Milieu1-03	
3	blanc milieu pos 01	
4	blanc milieu pos 02	
5	E2	
6	E3	
7	F2	
8	F3	
9	I1	
10	I2	

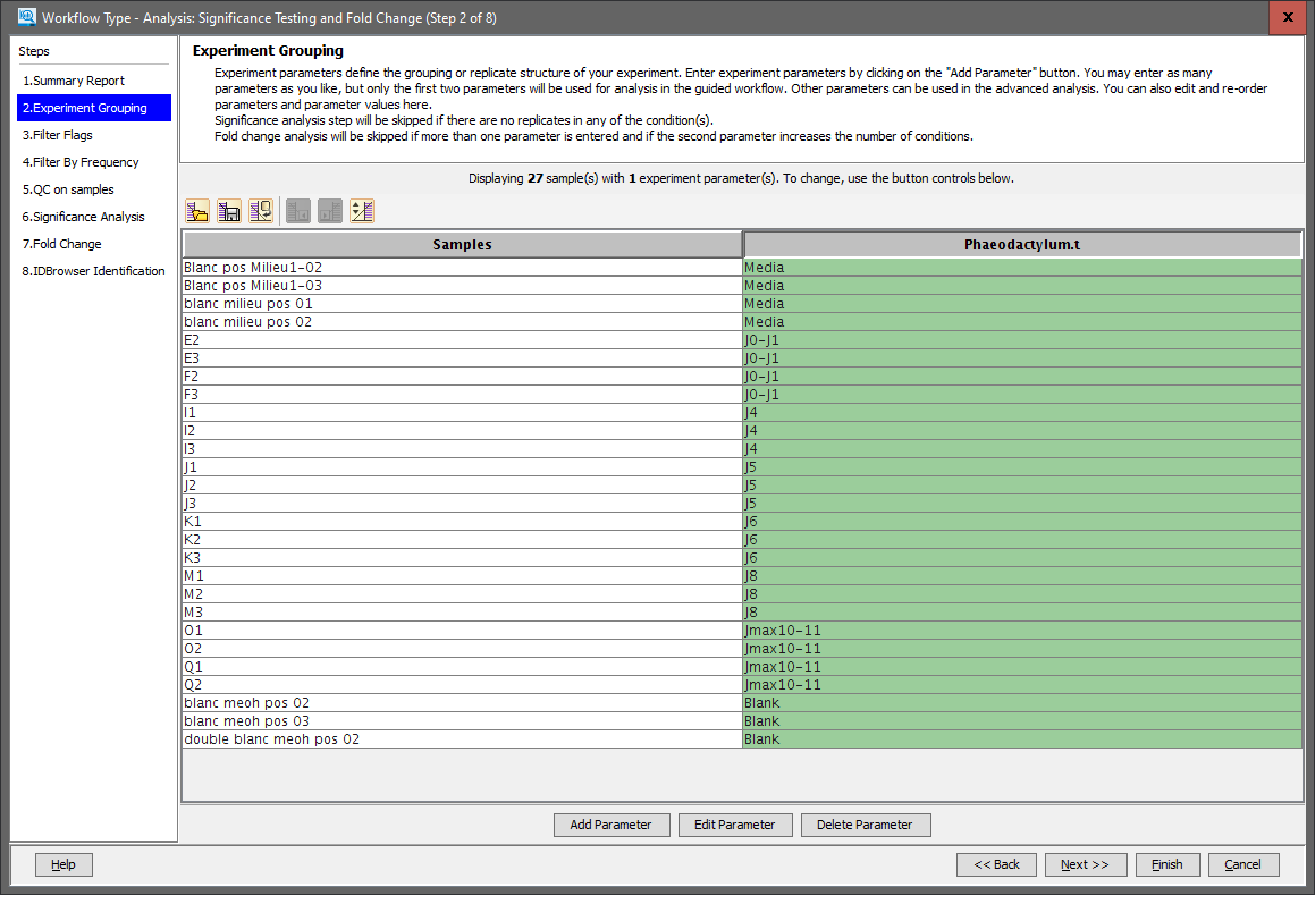


Workflow Type - Analysis: Significance Testing and Fold Change (Step 1 of 8)

Summary Report

The distribution of normalized intensity values across all samples is displayed in the Profile Plot.

MassHunterQual.IDENTIFIED_UNIDENTIFIED_COMPOUNDS experiment, No. of sample(s): **27**



Experiment Grouping

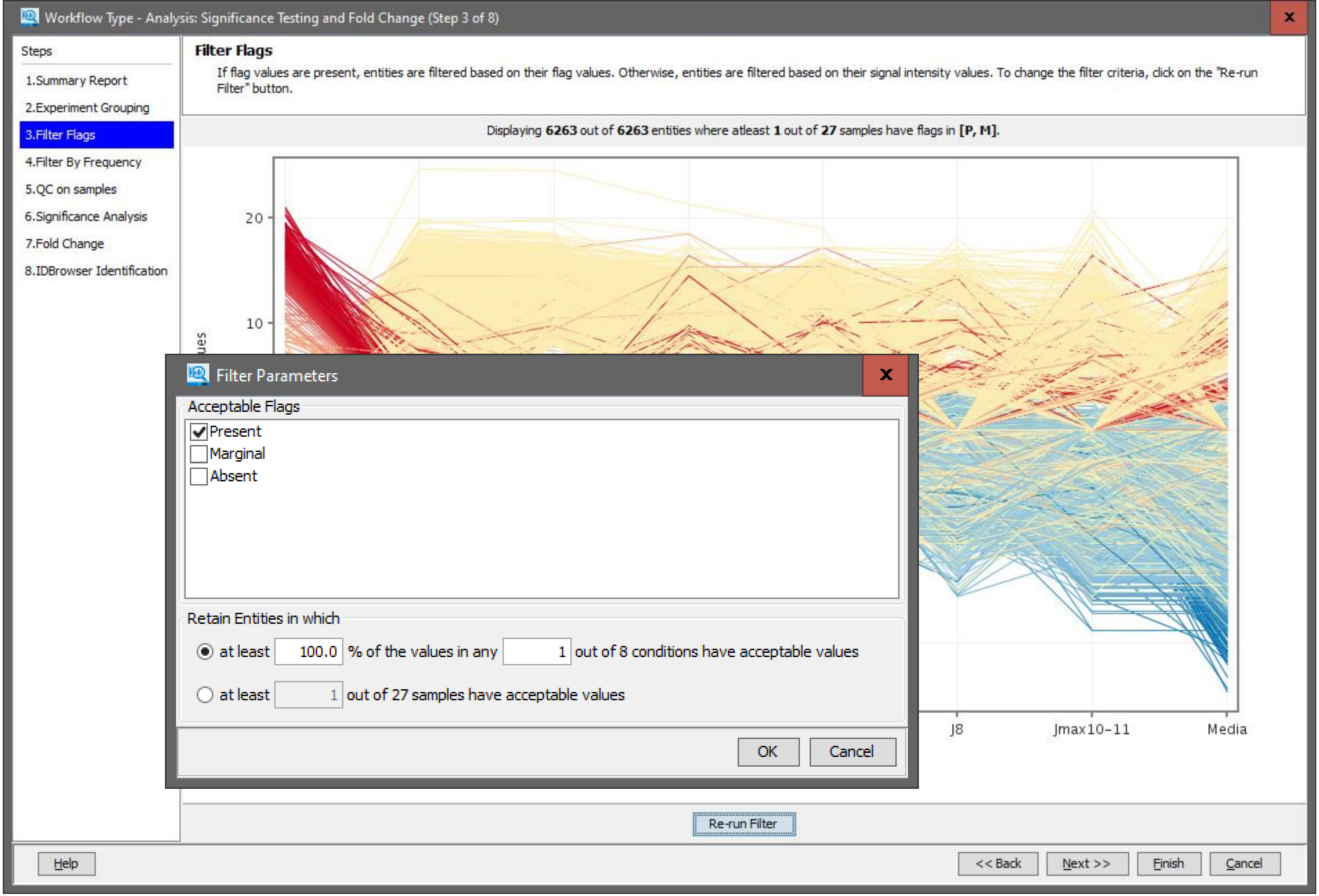
Experiment parameters define the grouping or replicate structure of your experiment. Enter experiment parameters by clicking on the "Add Parameter" button. You may enter as many parameters as you like, but only the first two parameters will be used for analysis in the guided workflow. Other parameters can be used in the advanced analysis. You can also edit and re-order parameters and parameter values here.

Significance analysis step will be skipped if there are no replicates in any of the condition(s).

Fold change analysis will be skipped if more than one parameter is entered and if the second parameter increases the number of conditions.

Displaying **27** sample(s) with **1** experiment parameter(s). To change, use the button controls below.

Samples	Phaeodactylum.t
Blanc pos Milieu1-02	Media
Blanc pos Milieu1-03	Media
blanc milieu pos 01	Media
blanc milieu pos 02	Media
E2	J0-J1
E3	J0-J1
F2	J0-J1
F3	J0-J1
I1	J4
I2	J4
I3	J4
J1	J5
J2	J5
J3	J5
K1	J6
K2	J6
K3	J6
M1	J8
M2	J8
M3	J8
O1	Jmax10-11
O2	Jmax10-11
Q1	Jmax10-11
Q2	Jmax10-11
blanc meoh pos 02	Blank
blanc meoh pos 03	Blank
double blanc meoh pos 02	Blank



Filter Flags

If flag values are present, entities are filtered based on their flag values. Otherwise, entities are filtered based on their signal intensity values. To change the filter criteria, click on the "Re-run Filter" button.

Displaying **6263** out of **6263** entities where atleast **1** out of **27** samples have flags in **[P, M]**.

Filter Parameters

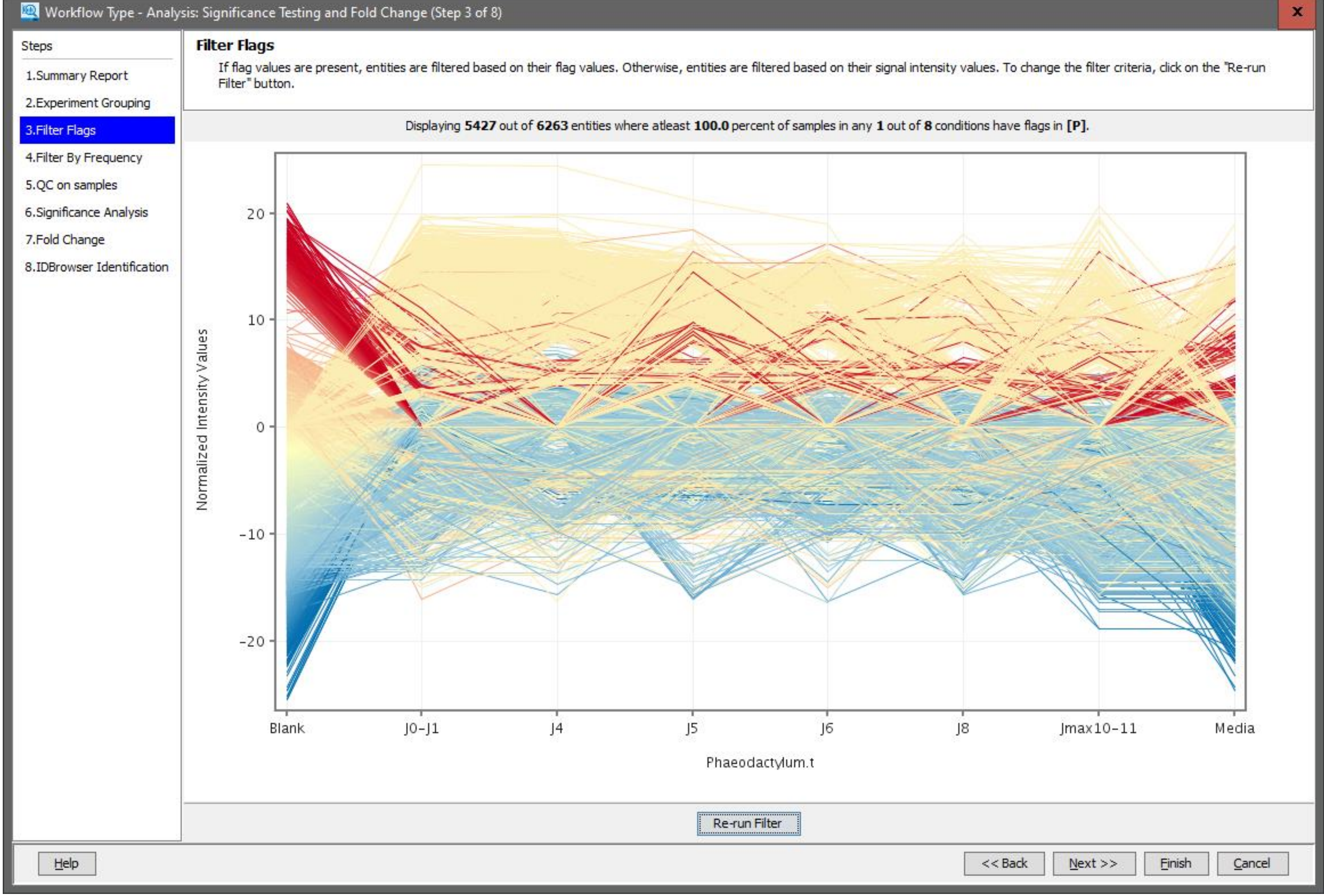
Acceptable Flags

☑ Present
☐ Marginal
☐ Absent

Retain Entities in which

● at least 100.0 % of the values in any 1 out of 8 conditions have acceptable values

○ at least 1 out of 27 samples have acceptable values

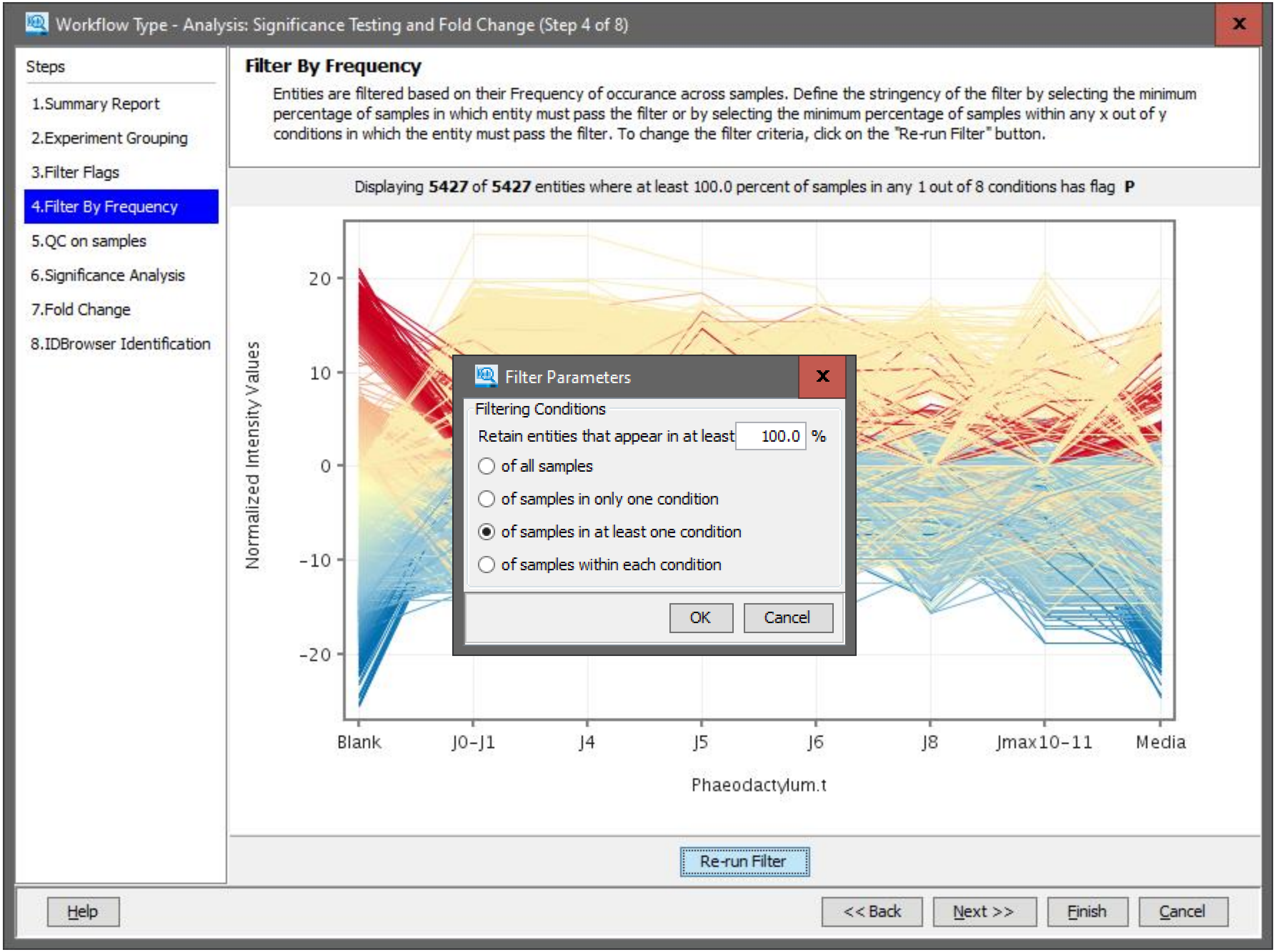


Workflow Type - Analysis: Significance Testing and Fold Change (Step 3 of 8)

Filter Flags

If flag values are present, entities are filtered based on their flag values. Otherwise, entities are filtered based on their signal intensity values. To change the filter criteria, click on the "Re-run Filter" button.

Displaying **5427** out of **6263** entities where atleast **100.0** percent of samples in any **1** out of **8** conditions have flags in **[P]**.



Workflow Type - Analysis: Significance Testing and Fold Change (Step 4 of 8)

Filter By Frequency

Entities are filtered based on their Frequency of occurance across samples. Define the stringency of the filter by selecting the minimum percentage of samples in which entity must pass the filter or by selecting the minimum percentage of samples within any x out of y conditions in which the entity must pass the filter. To change the filter criteria, click on the "Re-run Filter" button.

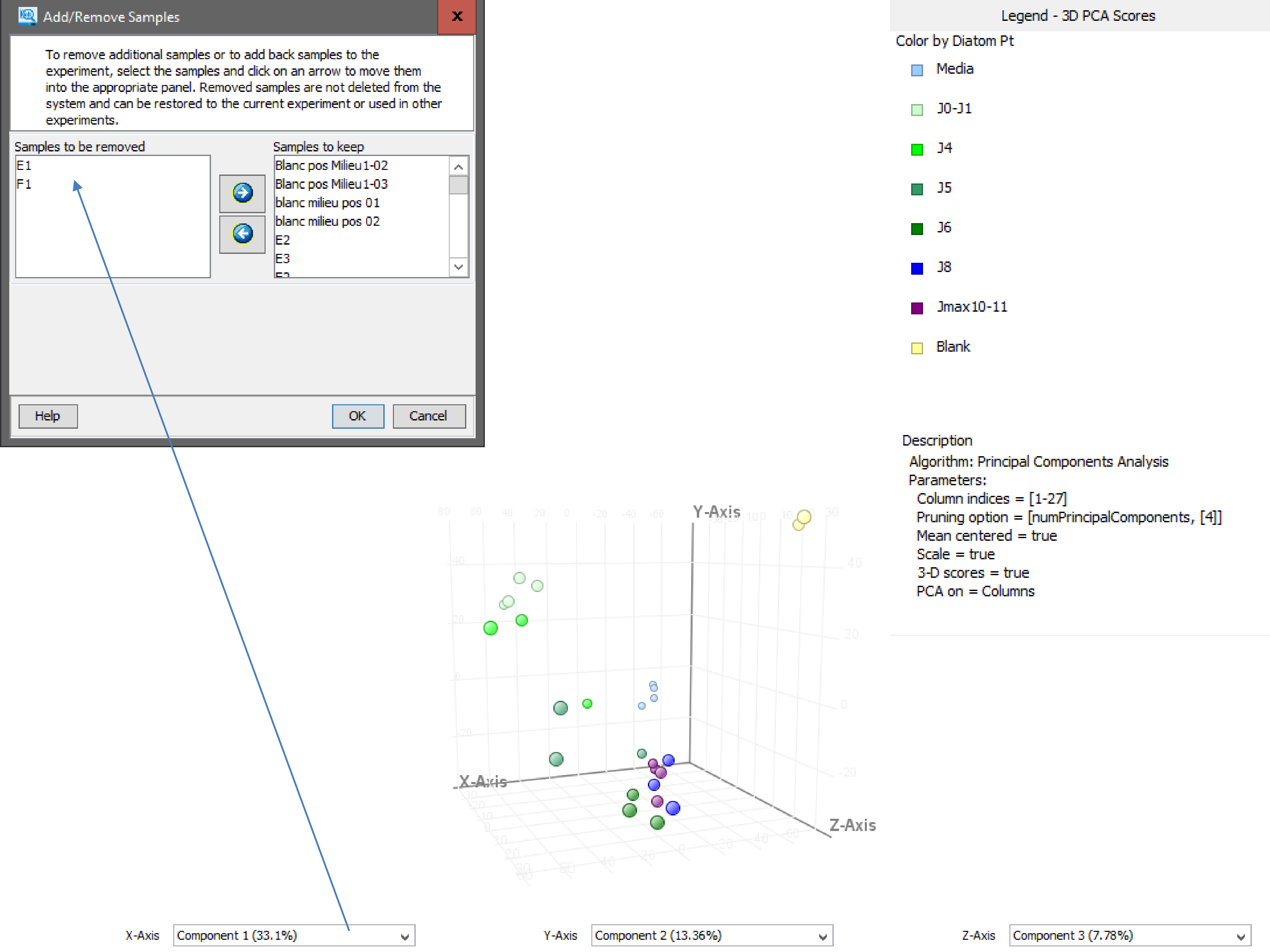
Displaying **5427** of **5427** entities where at least 100.0 percent of samples in any 1 out of 8 conditions has flag **P**

Filter Parameters

Filtering Conditions

Retain entities that appear in at least 100.0 %

○ of all samples
○ of samples in only one condition
● of samples in at least one condition
○ of samples within each condition



QC on samples

Sample quality can be assessed by examining the values in the PCA plot and other experiment specific quality plots.

Displaying **27** out of **27** samples retained in the analysis.

Samples	Phaeodactylum.t
Blanc pos Milieu1-02	Media
Blanc pos Milieu1-03	Media
blanc milieu pos 01	Media
blanc milieu pos 02	Media

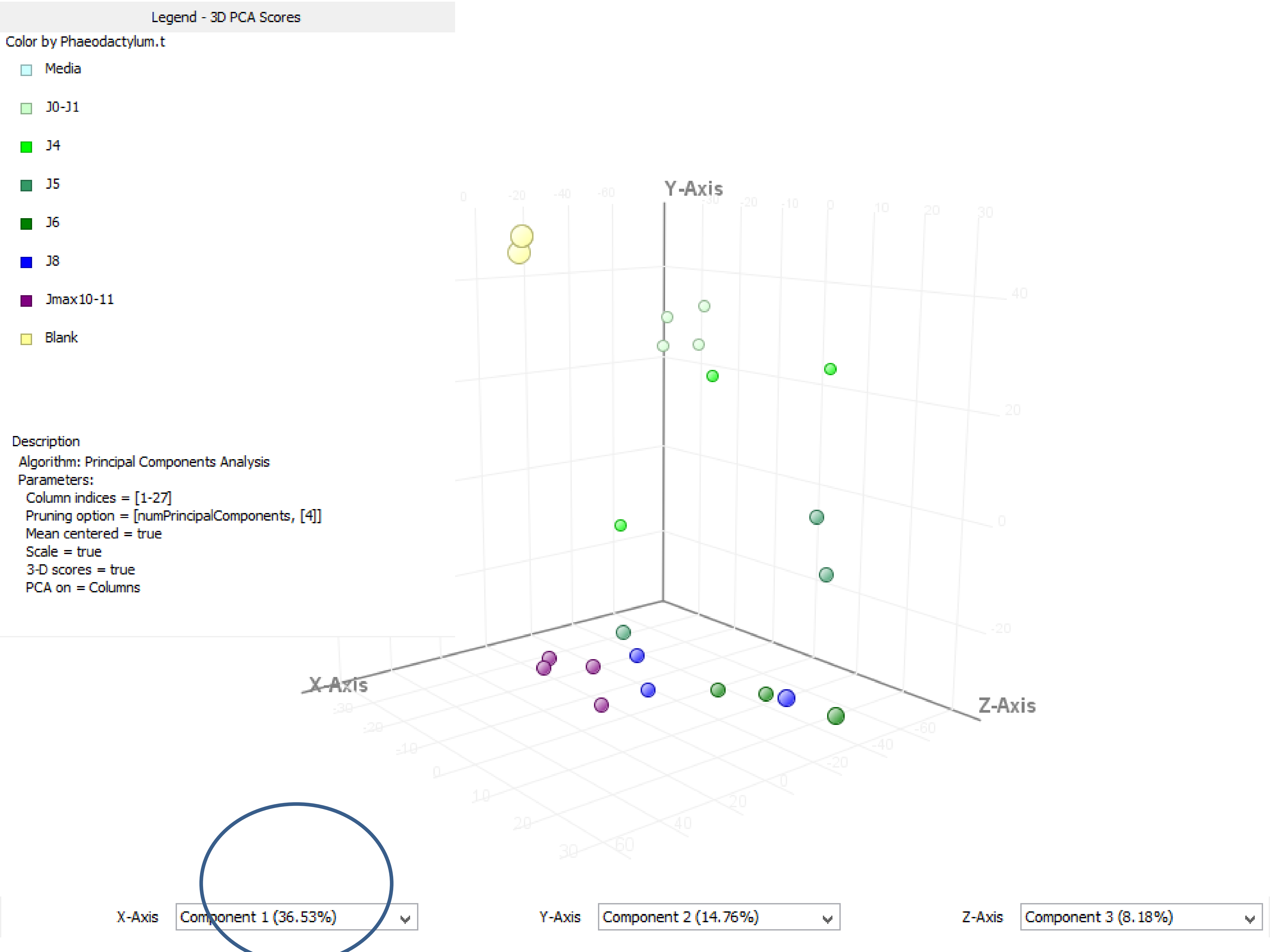
Legend - 3D PCA Scores

Color by Phaeodactylum.t

- 🟥 Media
- 🟨 J0-J1
- 🟦 J4
- ⬛ J5
- 🟩 J6
- 🟧 J8
- 🟦 Jmax10-11
- 🟥 Blank

Description
Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-27]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns

X-Axis Component 1 (36.53%)
Y-Axis Component 2 (14.76%)
Z-Axis Component 3 (8.18%)



Legend - 3D PCA Scores

Color by Phaeodactylum.t

- 🟦 Media
- 🟩 J0-J1
- 🟩 J4
- 🟩 J5
- 🟩 J6
- 🟦 J8
- 🟪 Jmax10-11
- 🟨 Blank

Description

Algorithm: Principal Components Analysis

Parameters:

Column indices = [1-27]

Pruning option = [numPrincipalComponents, [4]]

Mean centered = true

Scale = true

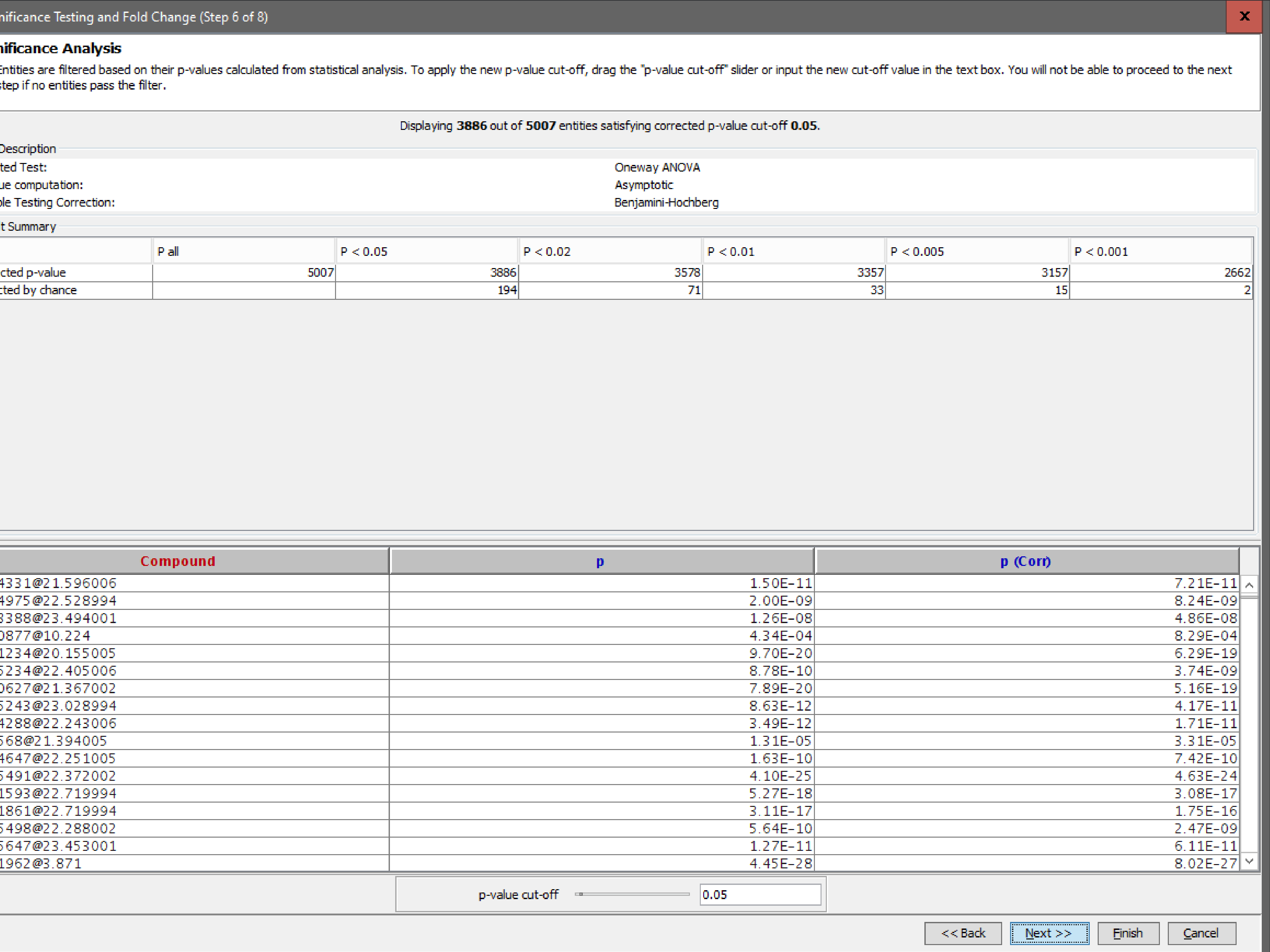
3-D scores = true

PCA on = Columns

X-Axis: Component 1 (36.53%)

Y-Axis: Component 2 (14.76%)

Z-Axis: Component 3 (8.18%)



nificance Testing and Fold Change (Step 6 of 8)

nificance Analysis

Entities are filtered based on their p-values calculated from statistical analysis. To apply the new p-value cut-off, drag the "p-value cut-off" slider or input the new cut-off value in the text box. You will not be able to proceed to the next step if no entities pass the filter.

Displaying **3886** out of **5007** entities satisfying corrected p-value cut-off **0.05**.

Description

ted Test: Oneway ANOVA

ue computation: Asymptotic

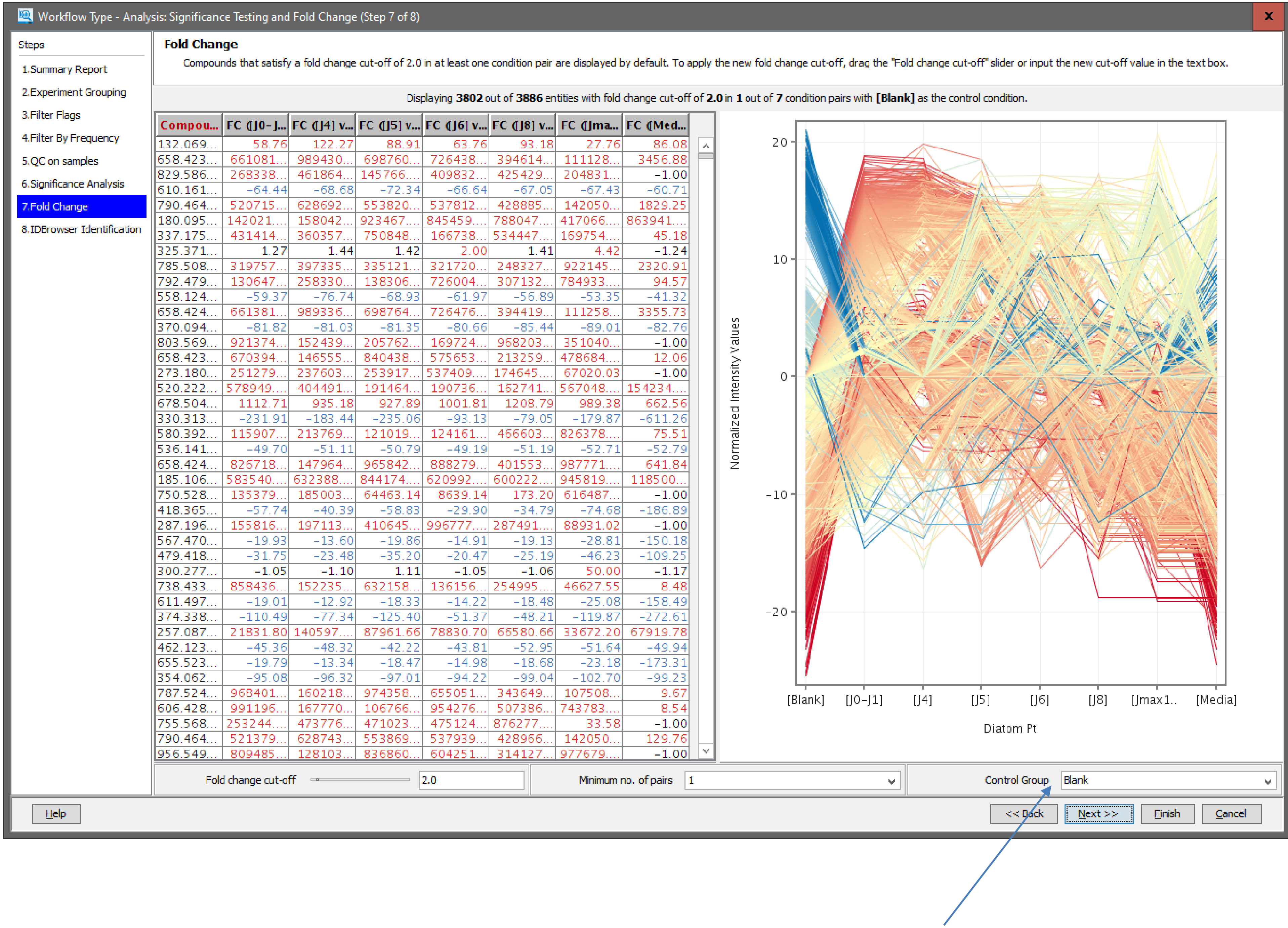
le Testing Correction: Benjamini-Hochberg

t Summary

	P all	P < 0.05	P < 0.02	P < 0.01	P < 0.005	P < 0.001
cted p-value	5007	3886	3578	3357	3157	2662
cted by chance		194	71	33	15	2

Compound	p	p (Corr)
4331@21.596006	1.50E-11	7.21E-11
4975@22.528994	2.00E-09	8.24E-09
3388@23.494001	1.26E-08	4.86E-08
0877@10.224	4.34E-04	8.29E-04
1234@20.155005	9.70E-20	6.29E-19
5234@22.405006	8.78E-10	3.74E-09
0627@21.367002	7.89E-20	5.16E-19
5243@23.028994	8.63E-12	4.17E-11
4288@22.243006	3.49E-12	1.71E-11
568@21.394005	1.31E-05	3.31E-05
4647@22.251005	1.63E-10	7.42E-10
5491@22.372002	4.10E-25	4.63E-24
1593@22.719994	5.27E-18	3.08E-17
1861@22.719994	3.11E-17	1.75E-16
5498@22.288002	5.64E-10	2.47E-09
5647@23.453001	1.27E-11	6.11E-11
1962@3.871	4.45E-28	8.02E-27

p-value cut-off: 0.05



Fold Change

Compounds that satisfy a fold change cut-off of 2.0 in at least one condition pair are displayed by default. To apply the new fold change cut-off, drag the "Fold change cut-off" slider or input the new cut-off value in the text box.

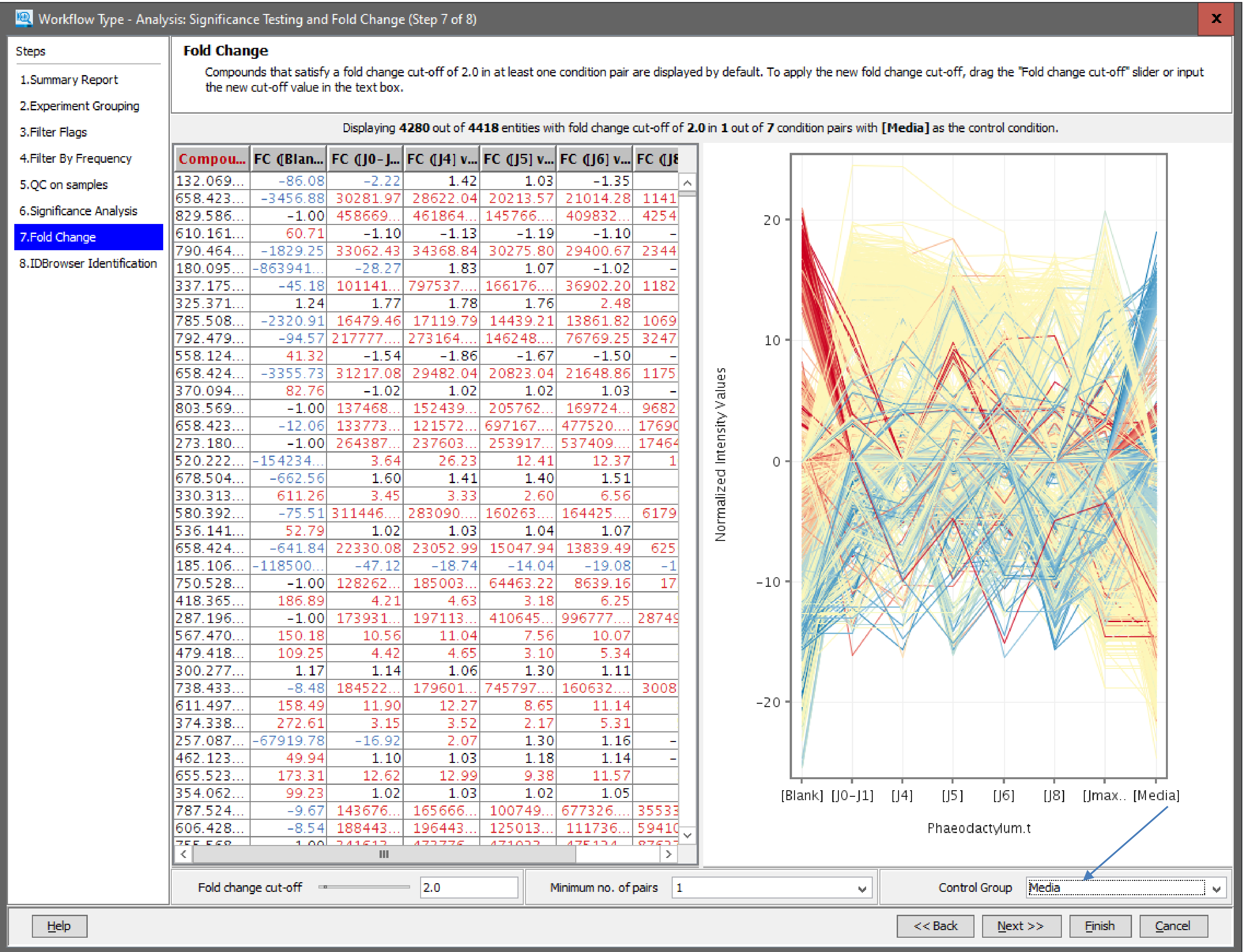
Displaying **3802** out of **3886** entities with fold change cut-off of **2.0** in **1** out of **7** condition pairs with **[Blank]** as the control condition.

Compou...	FC ([J0-J...	FC ([J4] v...	FC ([J5] v...	FC ([J6] v...	FC ([J8] v...	FC ([Jma...	FC ([Med...
132.069...	58.76	122.27	88.91	63.76	93.18	27.76	86.08
658.423...	661081...	989430...	698760...	726438...	394614...	111128...	3456.88
829.586...	268338...	461864...	145766....	409832...	425429...	204831...	-1.00
610.161...	-64.44	-68.68	-72.34	-66.64	-67.05	-67.43	-60.71
790.464...	520715...	628692...	553820...	537812...	428885...	142050...	1829.25
180.095...	142021....	158042...	923467....	845459....	788047....	417066....	863941....
337.175...	431414...	360357...	750848...	166738...	534447....	169754....	45.18
325.371...	1.27	1.44	1.42	2.00	1.41	4.42	-1.24
785.508...	319757...	397335...	335121...	321720...	248327...	922145...	2320.91
792.479...	130647...	258330...	138306...	726004...	307132...	784933....	94.57
558.124...	-59.37	-76.74	-68.93	-61.97	-56.89	-53.35	-41.32
658.424...	661381...	989336...	698764...	726476...	394419...	111258...	3355.73
370.094...	-81.82	-81.03	-81.35	-80.66	-85.44	-89.01	-82.76
803.569...	921374...	152439...	205762...	169724...	968203...	351040...	-1.00
658.423...	670394...	146555...	840438...	575653...	213259...	478684....	12.06
273.180...	251279...	237603...	253917...	537409....	174645....	67020.03	-1.00
520.222...	578949....	404491...	191464...	190736...	162741...	567048....	154234....
678.504...	1112.71	935.18	927.89	1001.81	1208.79	989.38	662.56
330.313...	-231.91	-183.44	-235.06	-93.13	-79.05	-179.87	-611.26
580.392...	115907...	213769...	121019...	124161...	466603...	826378....	75.51
536.141...	-49.70	-51.11	-50.79	-49.19	-51.19	-52.71	-52.79
658.424...	826718...	147964...	965842...	888279...	401553...	987771....	641.84
185.106...	583540....	632388....	844174....	620992....	600222....	945819....	118500...
750.528...	135379...	185003...	64463.14	8639.14	173.20	616487...	-1.00
418.365...	-57.74	-40.39	-58.83	-29.90	-34.79	-74.68	-186.89
287.196...	155816...	197113...	410645...	996777....	287491....	88931.02	-1.00
567.470...	-19.93	-13.60	-19.86	-14.91	-19.13	-28.81	-150.18
479.418...	-31.75	-23.48	-35.20	-20.47	-25.19	-46.23	-109.25
300.277...	-1.05	-1.10	1.11	-1.05	-1.06	50.00	-1.17
738.433...	858436...	152235...	632158...	136156...	254995....	46627.55	8.48
611.497...	-19.01	-12.92	-18.33	-14.22	-18.48	-25.08	-158.49
374.338...	-110.49	-77.34	-125.40	-51.37	-48.21	-119.87	-272.61
257.087...	21831.80	140597....	87961.66	78830.70	66580.66	33672.20	67919.78
462.123...	-45.36	-48.32	-42.22	-43.81	-52.95	-51.64	-49.94
655.523...	-19.79	-13.34	-18.47	-14.98	-18.68	-23.18	-173.31
354.062...	-95.08	-96.32	-97.01	-94.22	-99.04	-102.70	-99.23
787.524...	968401...	160218...	974358...	655051...	343649...	107508...	9.67
606.428...	991196...	167770...	106766...	954276...	507386...	743783....	8.54
755.568...	253244....	473776...	471023...	475124...	876277....	33.58	-1.00
790.464...	521379...	628743...	553869...	537939...	428966...	142050...	129.76
956.549...	809485...	128103...	836860...	604251...	314127...	977679....	-1.00

Fold change cut-off: 2.0

Minimum no. of pairs: 1

Control Group: Blank



Fold Change

Compounds that satisfy a fold change cut-off of 2.0 in at least one condition pair are displayed by default. To apply the new fold change cut-off, drag the "Fold change cut-off" slider or input the new cut-off value in the text box.

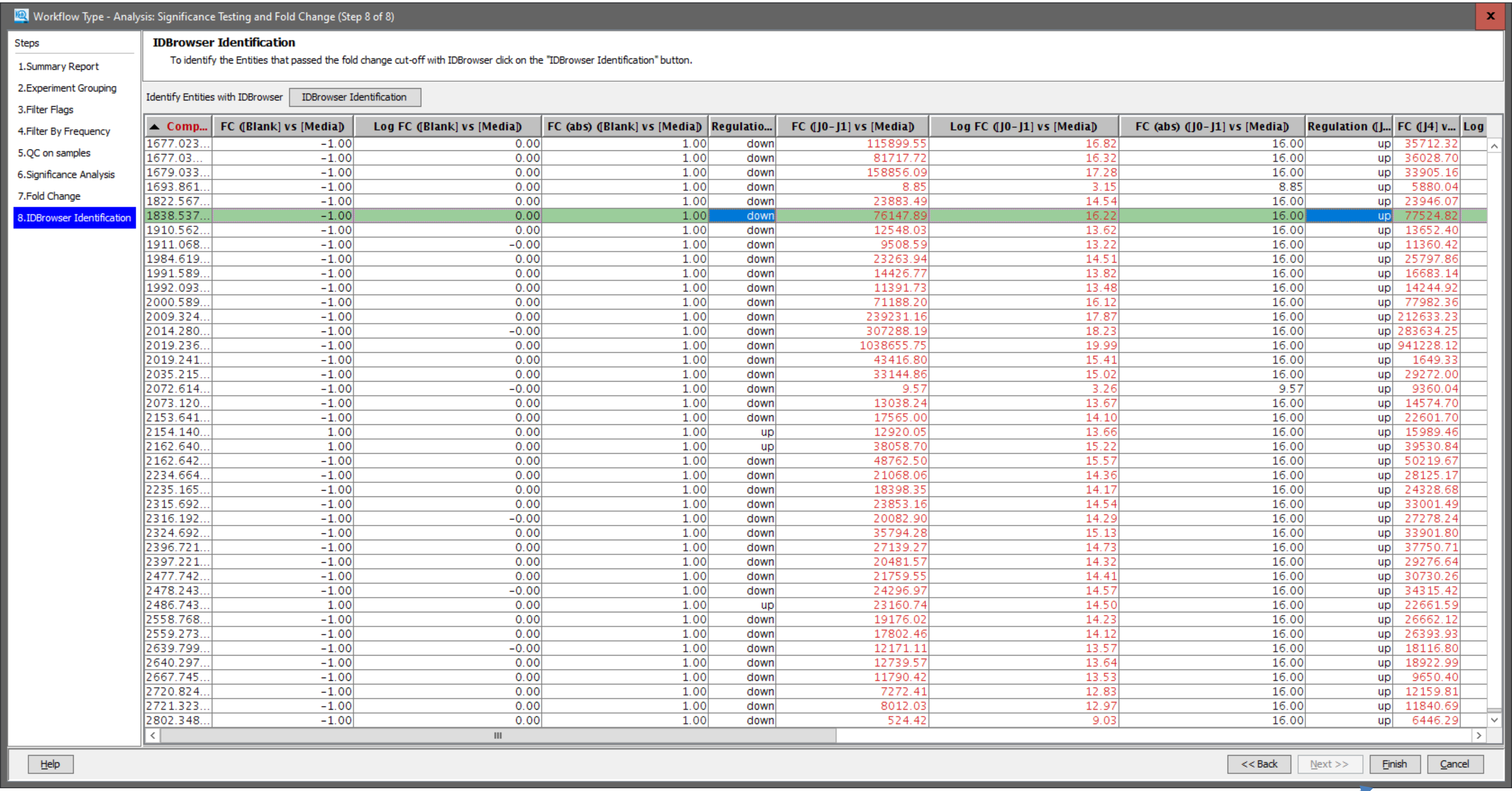
Displaying **4280** out of **4418** entities with fold change cut-off of **2.0** in **1** out of **7** condition pairs with **[Media]** as the control condition.

Compou...	FC ([Blan...	FC ([J0-J...	FC ([J4] v...	FC ([J5] v...	FC ([J6] v...	FC ([J8
132.069...	-86.08	-2.22	1.42	1.03	-1.35	
658.423...	-3456.88	30281.97	28622.04	20213.57	21014.28	1141
829.586...	-1.00	458669...	461864...	145766....	409832...	4254
610.161...	60.71	-1.10	-1.13	-1.19	-1.10	-
790.464...	-1829.25	33062.43	34368.84	30275.80	29400.67	2344
180.095...	-863941...	-28.27	1.83	1.07	-1.02	-
337.175...	-45.18	101141...	797537....	166176....	36902.20	1182
325.371...	1.24	1.77	1.78	1.76	2.48	
785.508...	-2320.91	16479.46	17119.79	14439.21	13861.82	1069
792.479...	-94.57	217777....	273164....	146248....	76769.25	3247
558.124...	41.32	-1.54	-1.86	-1.67	-1.50	-
658.424...	-3355.73	31217.08	29482.04	20823.04	21648.86	1175
370.094...	82.76	-1.02	1.02	1.02	1.03	-
803.569...	-1.00	137468...	152439...	205762...	169724...	9682
658.423...	-12.06	133773...	121572...	697167....	477520....	1769
273.180...	-1.00	264387...	237603...	253917...	537409....	17464
520.222...	-154234...	3.64	26.23	12.41	12.37	1
678.504...	-662.56	1.60	1.41	1.40	1.51	
330.313...	611.26	3.45	3.33	2.60	6.56	
580.392...	-75.51	311446....	283090....	160263....	164425....	6179
536.141...	52.79	1.02	1.03	1.04	1.07	
658.424...	-641.84	22330.08	23052.99	15047.94	13839.49	625
185.106...	-118500...	-47.12	-18.74	-14.04	-19.08	-1
750.528...	-1.00	128262...	185003...	64463.22	8639.16	17
418.365...	186.89	4.21	4.63	3.18	6.25	
287.196...	-1.00	173931...	197113...	410645...	996777....	2874
567.470...	150.18	10.56	11.04	7.56	10.07	
479.418...	109.25	4.42	4.65	3.10	5.34	
300.277...	1.17	1.14	1.06	1.30	1.11	
738.433...	-8.48	184522...	179601...	745797....	160632....	3008
611.497...	158.49	11.90	12.27	8.65	11.14	
374.338...	272.61	3.15	3.52	2.17	5.31	
257.087...	-67919.78	-16.92	2.07	1.30	1.16	-
462.123...	49.94	1.10	1.03	1.18	1.14	-
655.523...	173.31	12.62	12.99	9.38	11.57	
354.062...	99.23	1.02	1.03	1.02	1.05	
787.524...	-9.67	143676...	165666...	100749...	677326....	3553
606.428...	-8.54	188443...	196443...	125013...	111736...	5941

Fold change cut-off: 2.0

Minimum no. of pairs: 1

Control Group: Media



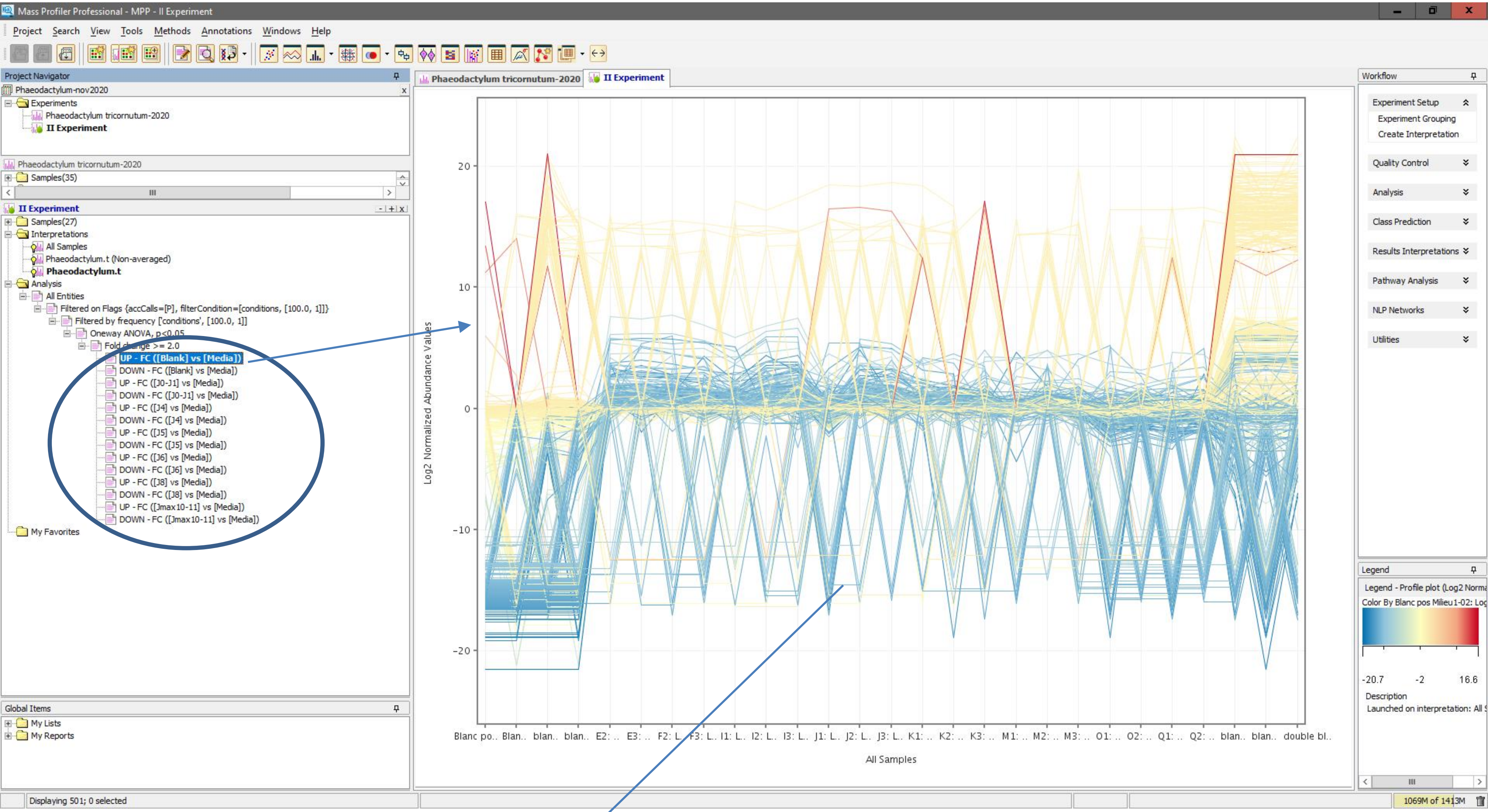
IDBrowser Identification

To identify the Entities that passed the fold change cut-off with IDBrowser click on the "IDBrowser Identification" button.

Identify Entities with IDBrowser [IDBrowser Identification]

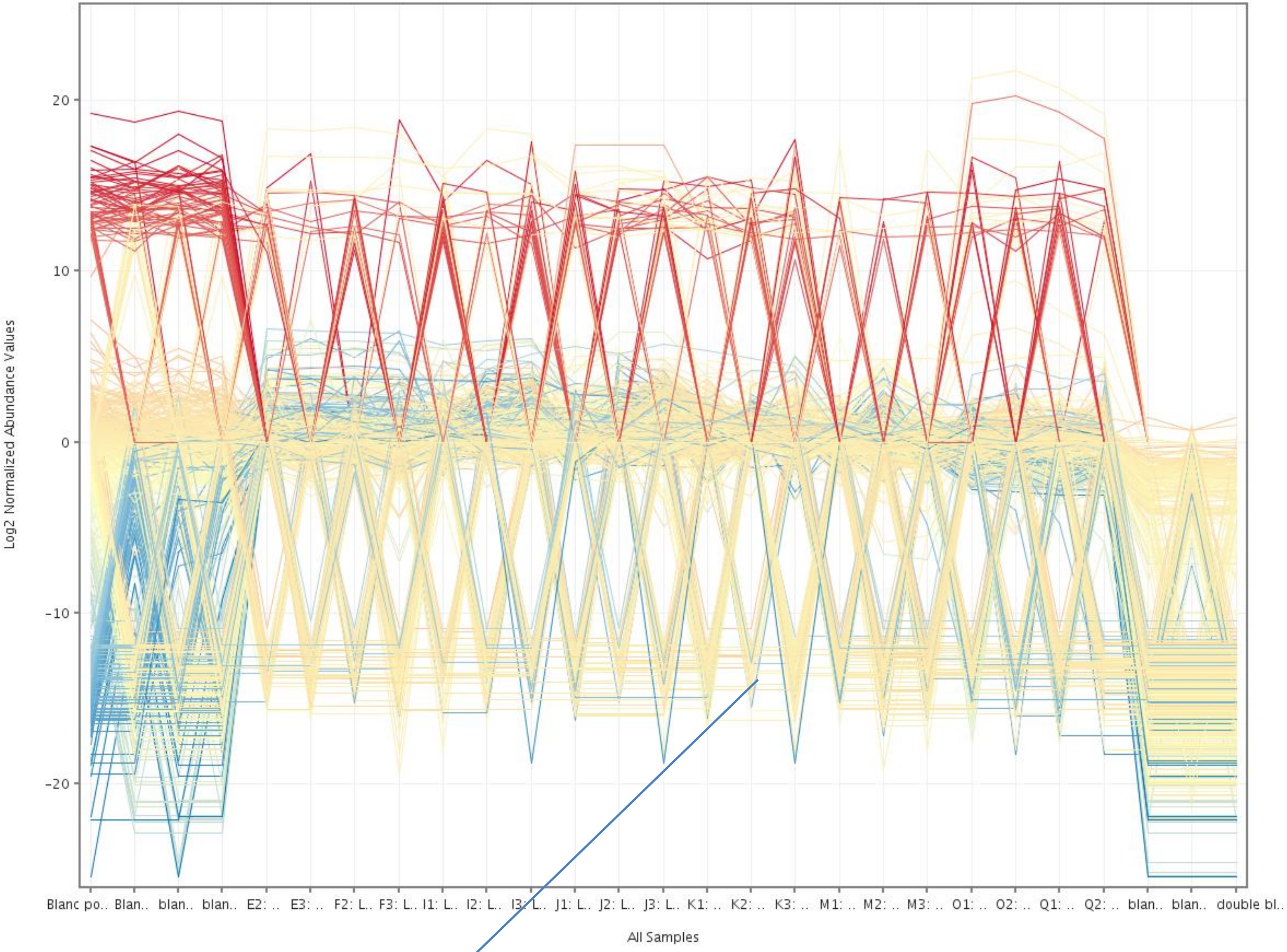
▲ Comp...	FC ([Blank] vs [Media])	Log FC ([Blank] vs [Media])	FC (abs) ([Blank] vs [Media])	Regulatio...	FC ([J0-J1] vs [Media])	Log FC ([J0-J1] vs [Media])	FC (abs) ([J0-J1] vs [Media])	Regulation ([J...	FC ([J4] v...	Log
1677.023...	-1.00	0.00	1.00	down	115899.55	16.82	16.00	up	35712.32	
1677.03...	-1.00	0.00	1.00	down	81717.72	16.32	16.00	up	36028.70	
1679.033...	-1.00	0.00	1.00	down	158856.09	17.28	16.00	up	33905.16	
1693.861...	-1.00	0.00	1.00	down	8.85	3.15	8.85	up	5880.04	
1822.567...	-1.00	0.00	1.00	down	23883.49	14.54	16.00	up	23946.07	
1838.537...	-1.00	0.00	1.00	down	76147.89	16.22	16.00	up	77524.82	
1910.562...	-1.00	0.00	1.00	down	12548.03	13.62	16.00	up	13652.40	
1911.068...	-1.00	-0.00	1.00	down	9508.59	13.22	16.00	up	11360.42	
1984.619...	-1.00	0.00	1.00	down	23263.94	14.51	16.00	up	25797.86	
1991.589...	-1.00	0.00	1.00	down	14426.77	13.82	16.00	up	16683.14	
1992.093...	-1.00	0.00	1.00	down	11391.73	13.48	16.00	up	14244.92	
2000.589...	-1.00	0.00	1.00	down	71188.20	16.12	16.00	up	77982.36	
2009.324...	-1.00	0.00	1.00	down	239231.16	17.87	16.00	up	212633.23	
2014.280...	-1.00	-0.00	1.00	down	307288.19	18.23	16.00	up	283634.25	
2019.236...	-1.00	0.00	1.00	down	1038655.75	19.99	16.00	up	941228.12	
2019.241...	-1.00	0.00	1.00	down	43416.80	15.41	16.00	up	1649.33	
2035.215...	-1.00	0.00	1.00	down	33144.86	15.02	16.00	up	29272.00	
2072.614...	-1.00	-0.00	1.00	down	9.57	3.26	9.57	up	9360.04	
2073.120...	-1.00	0.00	1.00	down	13038.24	13.67	16.00	up	14574.70	
2153.641...	-1.00	0.00	1.00	down	17565.00	14.10	16.00	up	22601.70	
2154.140...	1.00	0.00	1.00	up	12920.05	13.66	16.00	up	15989.46	
2162.640...	1.00	0.00	1.00	up	38058.70	15.22	16.00	up	39530.84	
2162.642...	-1.00	0.00	1.00	down	48762.50	15.57	16.00	up	50219.67	
2234.664...	-1.00	0.00	1.00	down	21068.06	14.36	16.00	up	28125.17	
2235.165...	-1.00	0.00	1.00	down	18398.35	14.17	16.00	up	24328.68	
2315.692...	-1.00	0.00	1.00	down	23853.16	14.54	16.00	up	33001.49	
2316.192...	-1.00	-0.00	1.00	down	20082.90	14.29	16.00	up	27278.24	
2324.692...	-1.00	0.00	1.00	down	35794.28	15.13	16.00	up	33901.80	
2396.721...	-1.00	0.00	1.00	down	27139.27	14.73	16.00	up	37750.71	
2397.221...	-1.00	0.00	1.00	down	20481.57	14.32	16.00	up	29276.64	
2477.742...	-1.00	0.00	1.00	down	21759.55	14.41	16.00	up	30730.26	
2478.243...	-1.00	-0.00	1.00	down	24296.97	14.57	16.00	up	34315.42	
2486.743...	1.00	0.00	1.00	up	23160.74	14.50	16.00	up	22661.59	
2558.768...	-1.00	0.00	1.00	down	19176.02	14.23	16.00	up	26662.12	
2559.273...	-1.00	0.00	1.00	down	17802.46	14.12	16.00	up	26393.93	
2639.799...	-1.00	-0.00	1.00	down	12171.11	13.57	16.00	up	18116.80	
2640.297...	-1.00	0.00	1.00	down	12739.57	13.64	16.00	up	18922.99	
2667.745...	-1.00	0.00	1.00	down	11790.42	13.53	16.00	up	9650.40	
2720.824...	-1.00	0.00	1.00	down	7272.41	12.83	16.00	up	12159.81	
2721.323...	-1.00	0.00	1.00	down	8012.03	12.97	16.00	up	11840.69	
2802.348...	-1.00	0.00	1.00	down	524.42	9.03	16.00	up	6446.29	

Fichier exporté dans Excel et envoyé chez vous

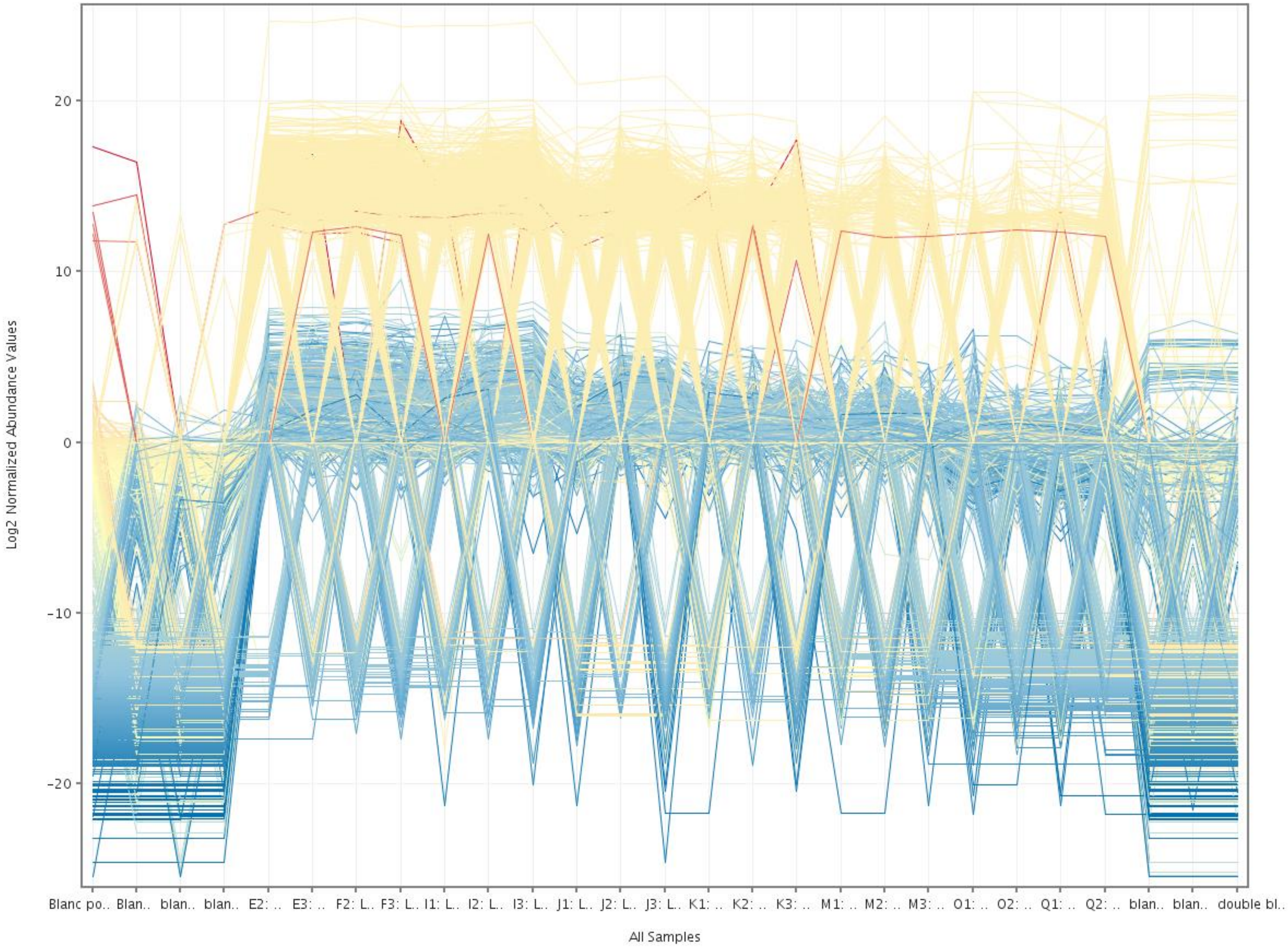


On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 501 métabolites UP - FC ([Blank] vs [Media])

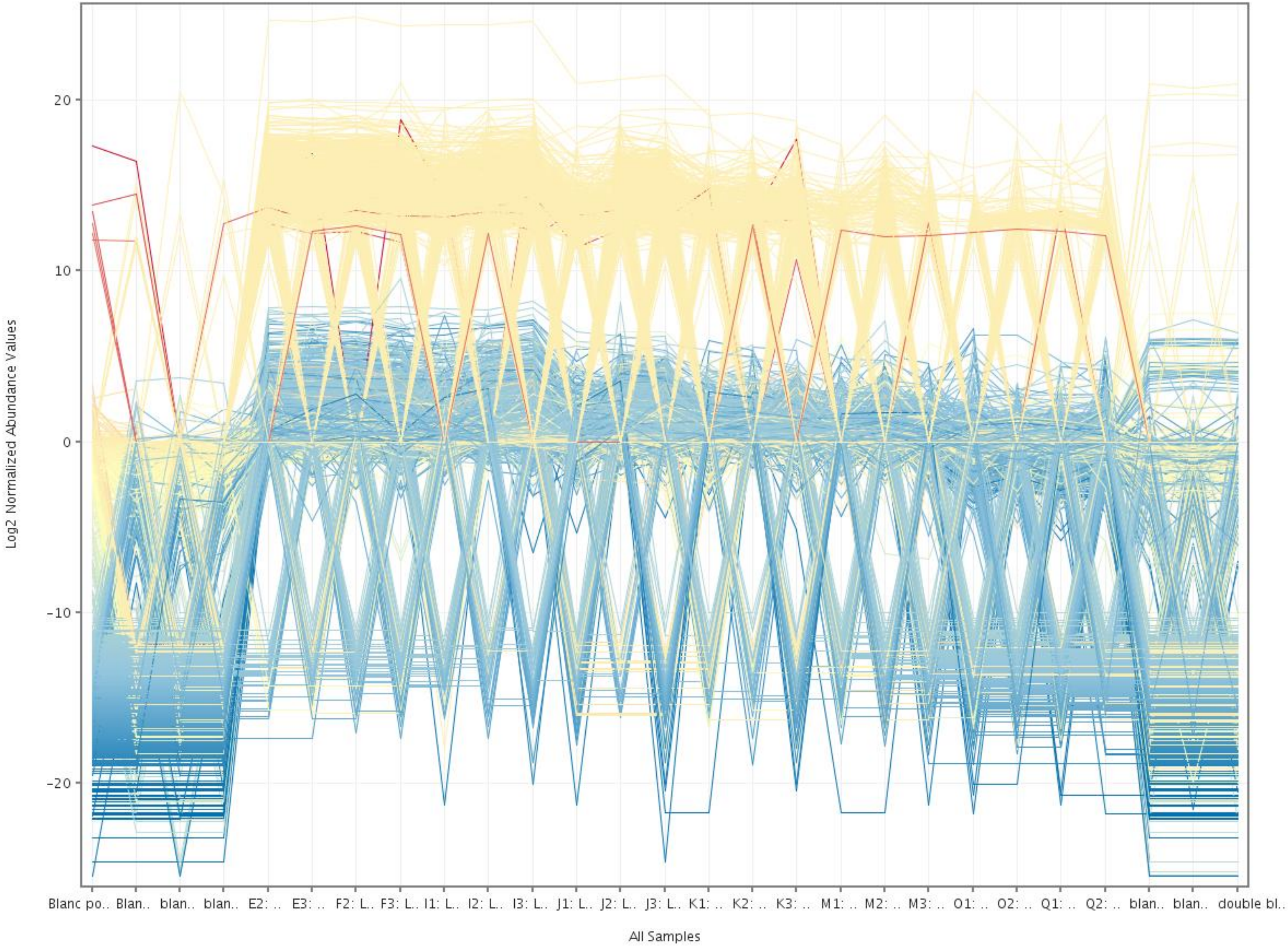


On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 1381 métabolites DOWN - FC ([Blank] vs [Media])



On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 2956 métabolites UP - FC ([J0-J1] vs [Media])

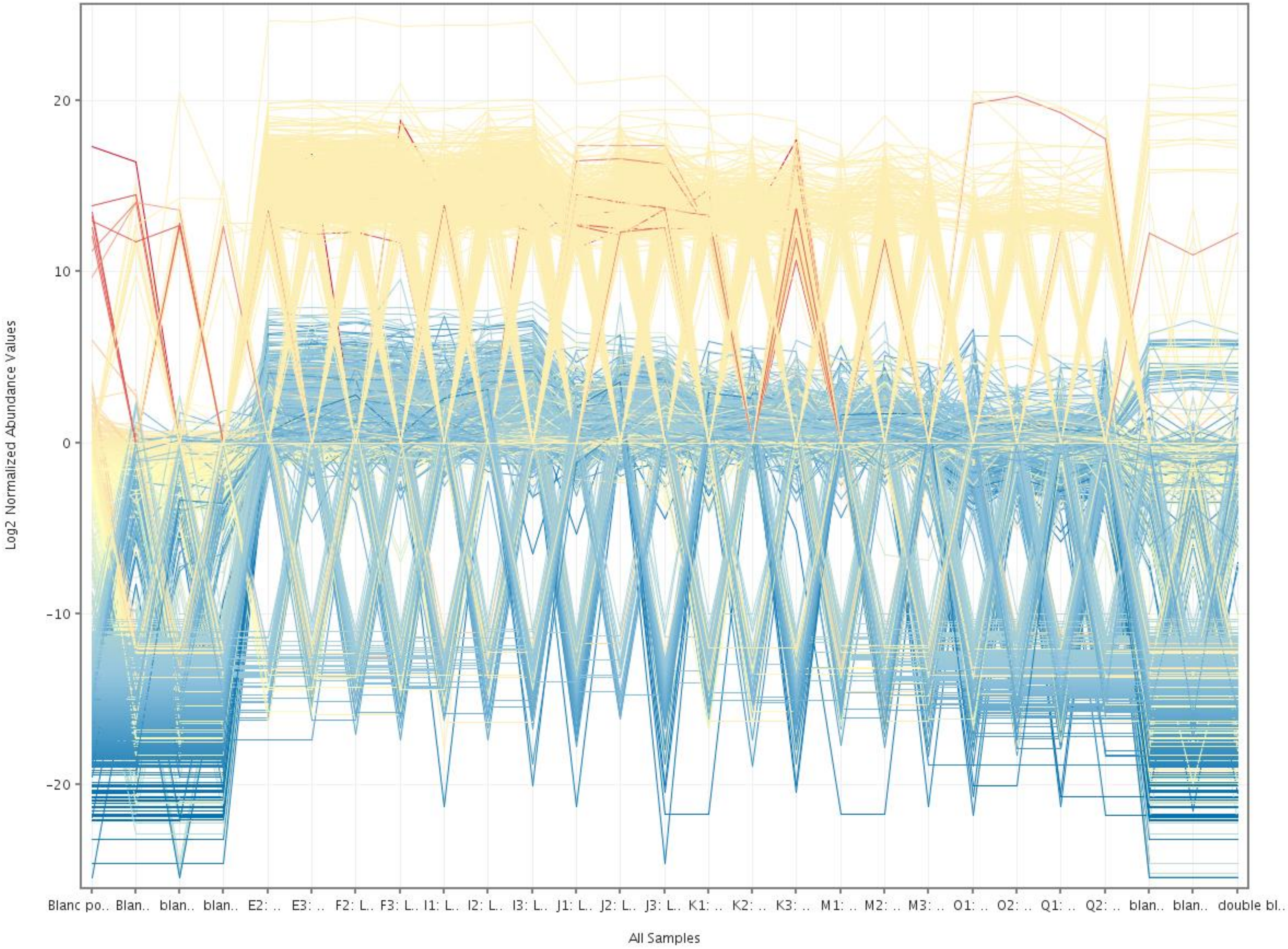
On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 378 métabolites DOWN - FC ([J0-J1] vs [Media])



On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé
Ici les 3048 métabolites UP - FC ([J4] vs [Media])

On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

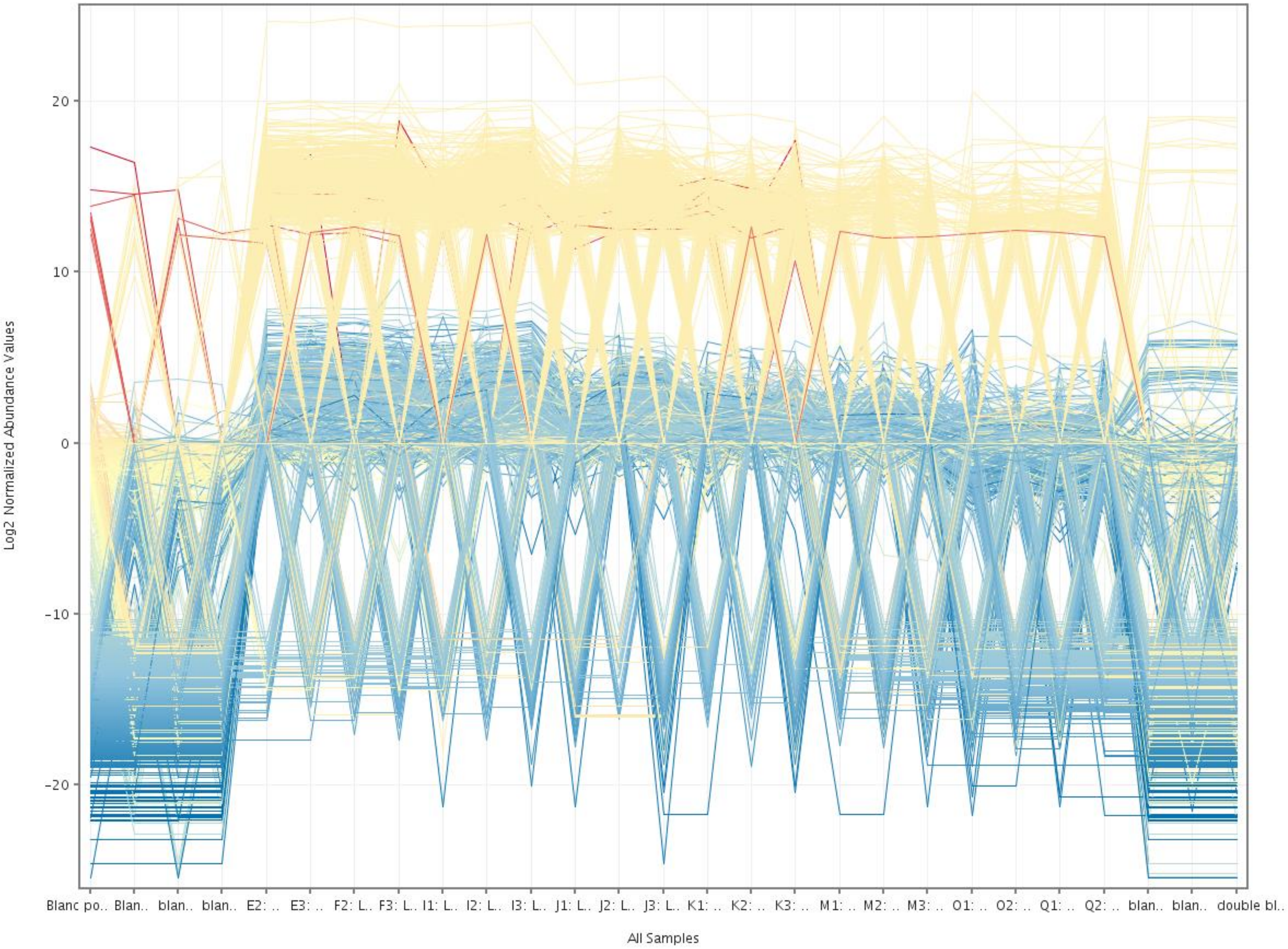
Ici les 272 métabolites DOWN - FC ([J4] vs [Media])



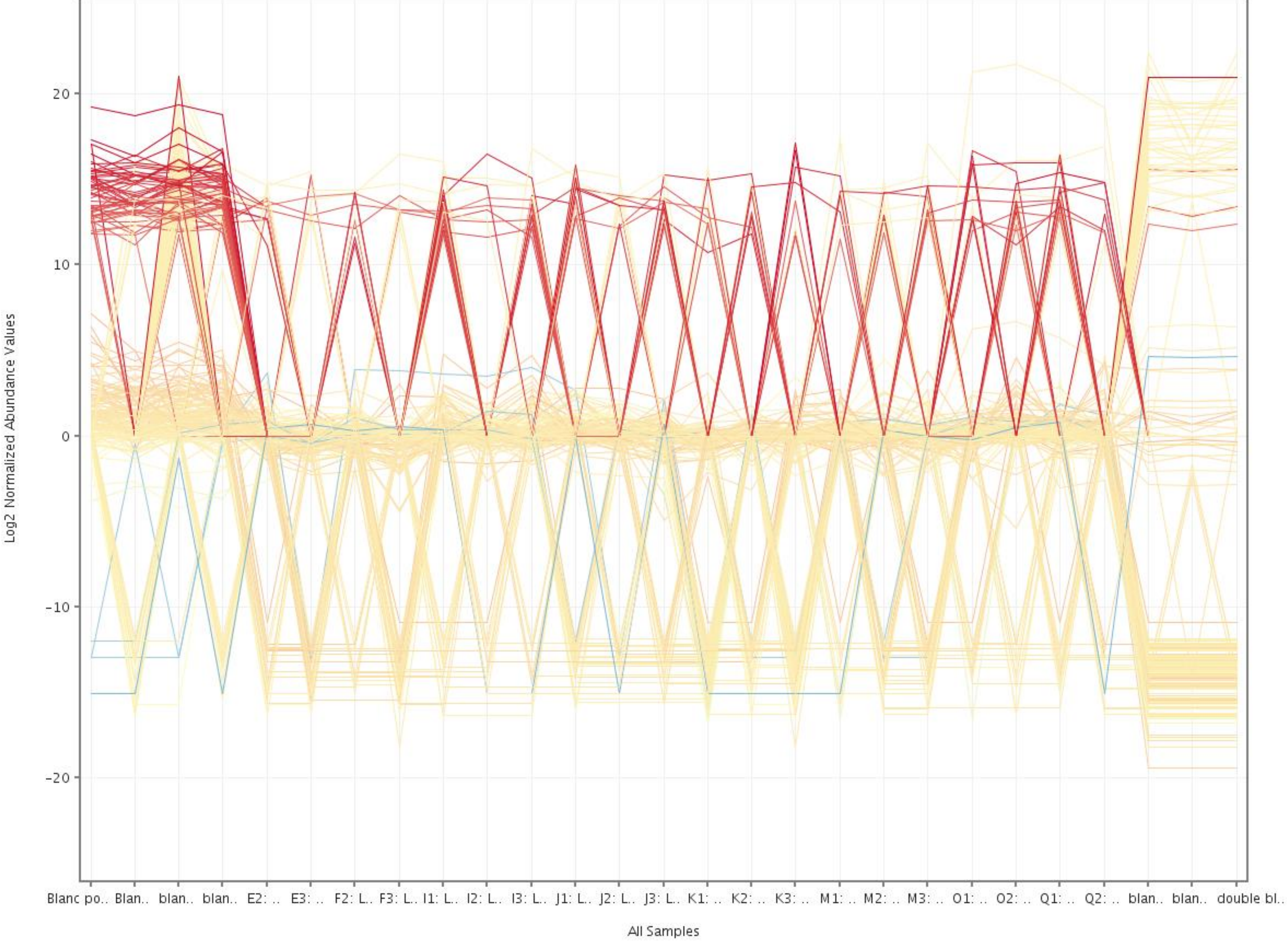
On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 3035 métabolites UP - FC ([J5] vs [Media])

On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

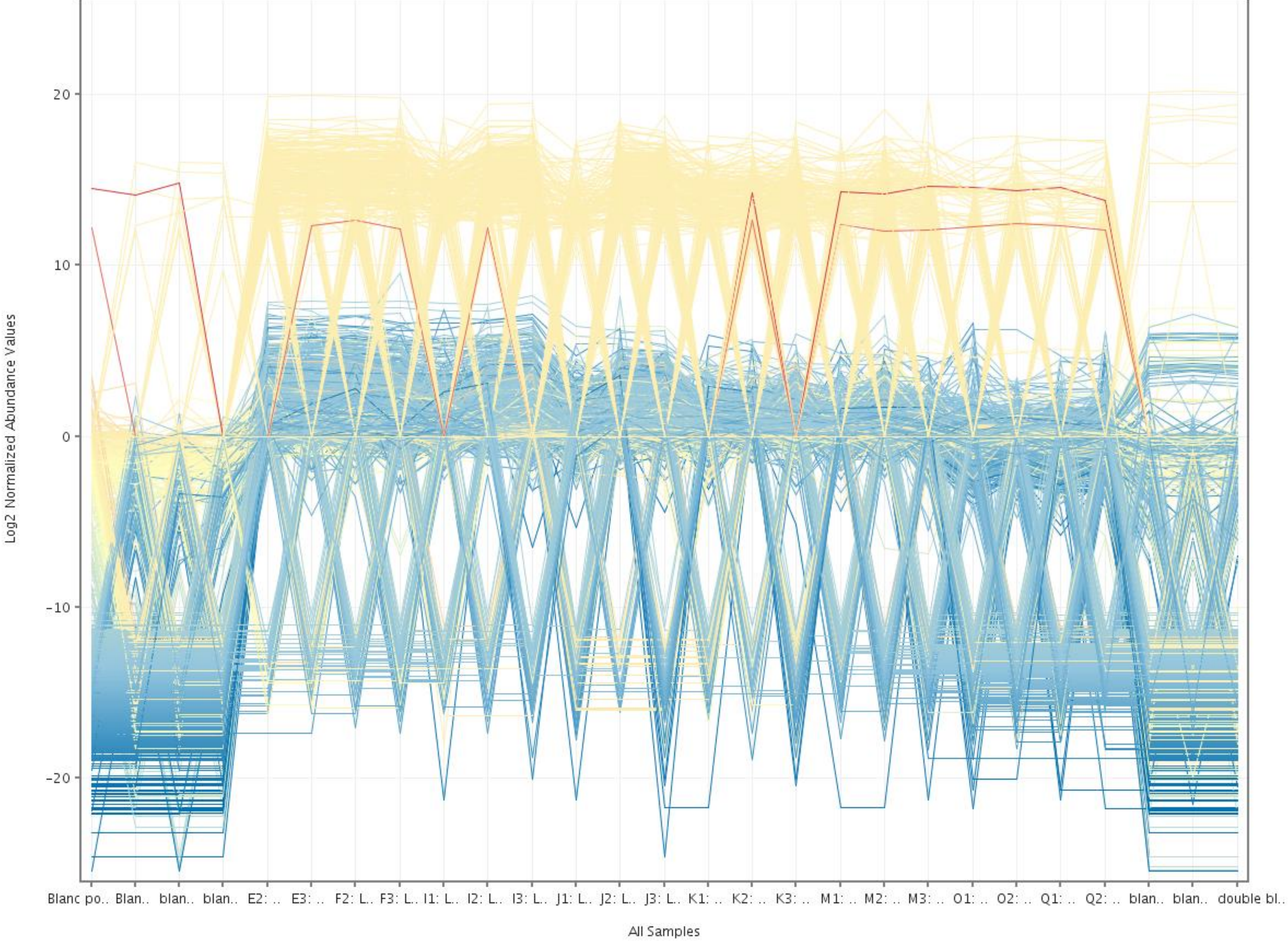
Ici les 259 métabolites DOWN - FC ([J5] vs [Media])



On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 2739 métabolites UP - FC ([J6] vs [Media])

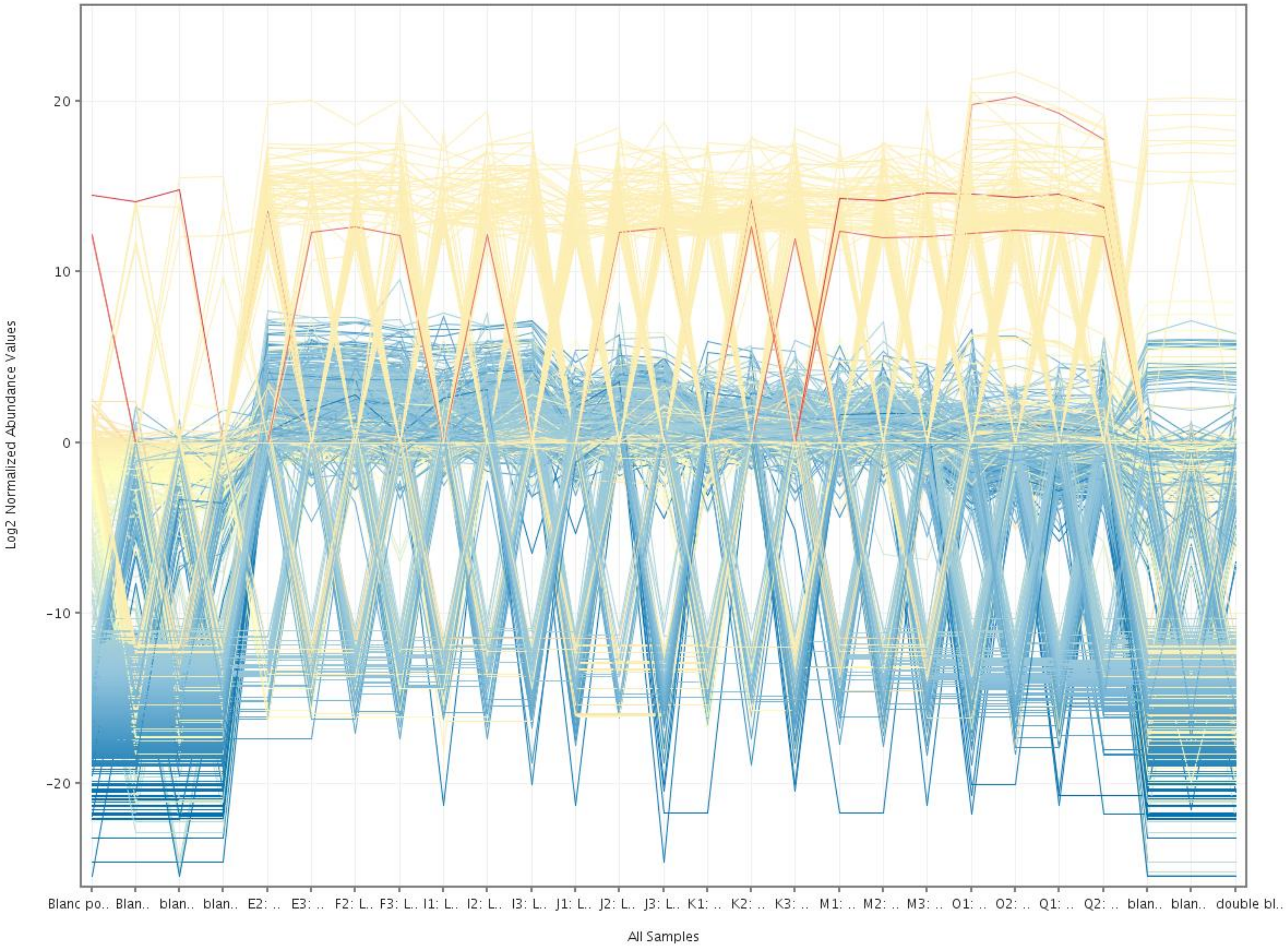


On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 242 métabolites DOWN - FC ([J6] vs [Media])

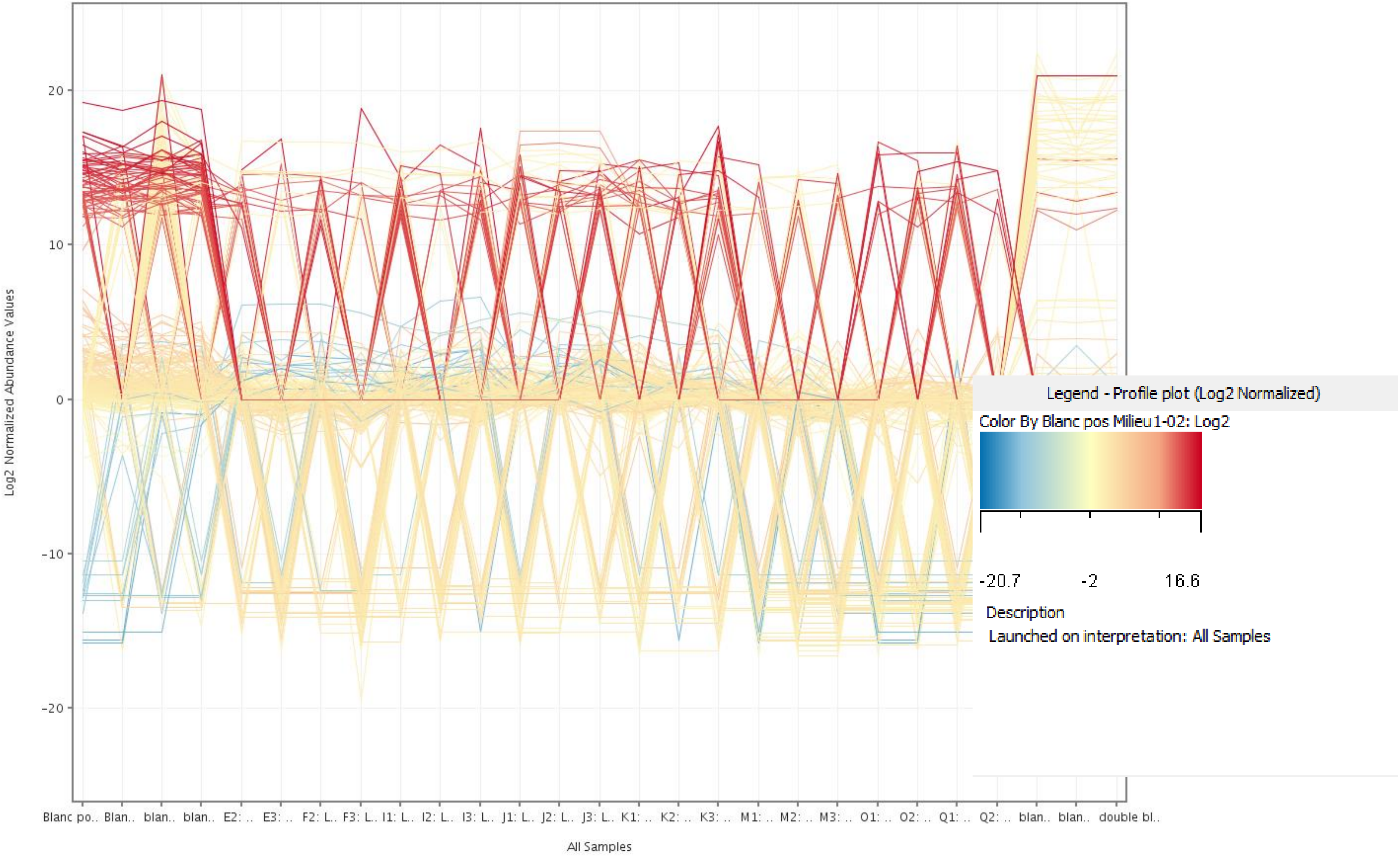


On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 2304 métabolites UP - FC ([J8] vs [Media])

On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 389 métabolites DOWN - FC ([J8] vs [Media])



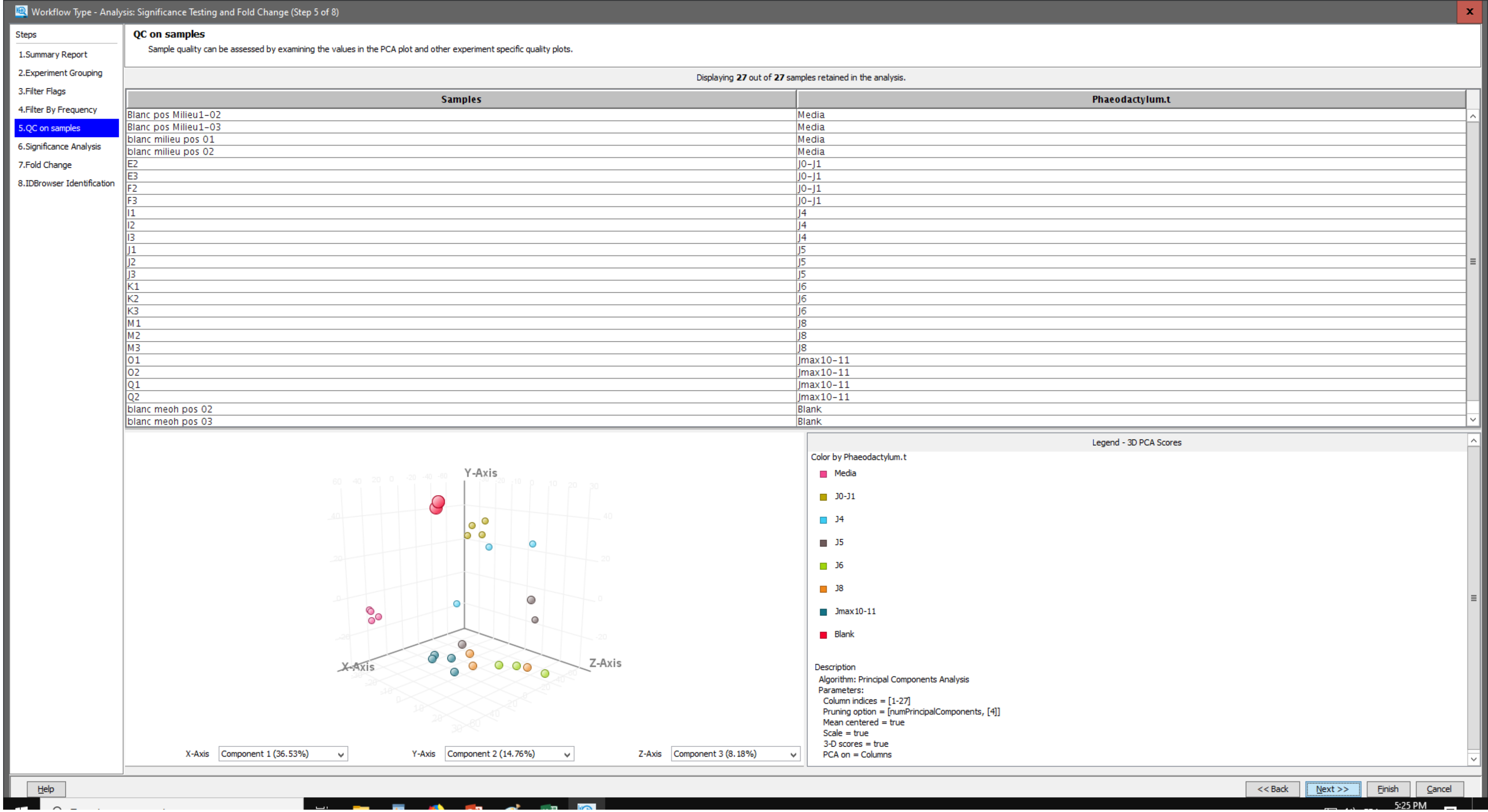
On obtient alors la cinétique de chaque métabolites
exprimé vs sous exprimé
Ici les 1941 métabolites UP - FC ([Jmax10-11] vs [Media])



On obtient alors la cinétique de chaque métabolites exprimé vs sous exprimé

Ici les 329 métabolites DOWN - FC ([Jmax10-11] vs [Media])

SUITE III



QC on samples

Sample quality can be assessed by examining the values in the PCA plot and other experiment specific quality plots.

Displaying **27** out of **27** samples retained in the analysis.

Samples	Phaeodactylum.t
Blanc pos Milieu1-02	Media
Blanc pos Milieu1-03	Media
blanc milieu pos 01	Media
blanc milieu pos 02	Media
E2	J0-J1
E3	J0-J1
F2	J0-J1
F3	J0-J1
I1	J4
I2	J4
I3	J4
J1	J5
J2	J5
J3	J5
K1	J6
K2	J6
K3	J6
M1	J8
M2	J8
M3	J8
O1	Jmax10-11
O2	Jmax10-11
Q1	Jmax10-11
Q2	Jmax10-11
blanc meoh pos 02	Blank
blanc meoh pos 03	Blank

X-Axis Component 1 (36.53%)
Y-Axis Component 2 (14.76%)
Z-Axis Component 3 (8.18%)

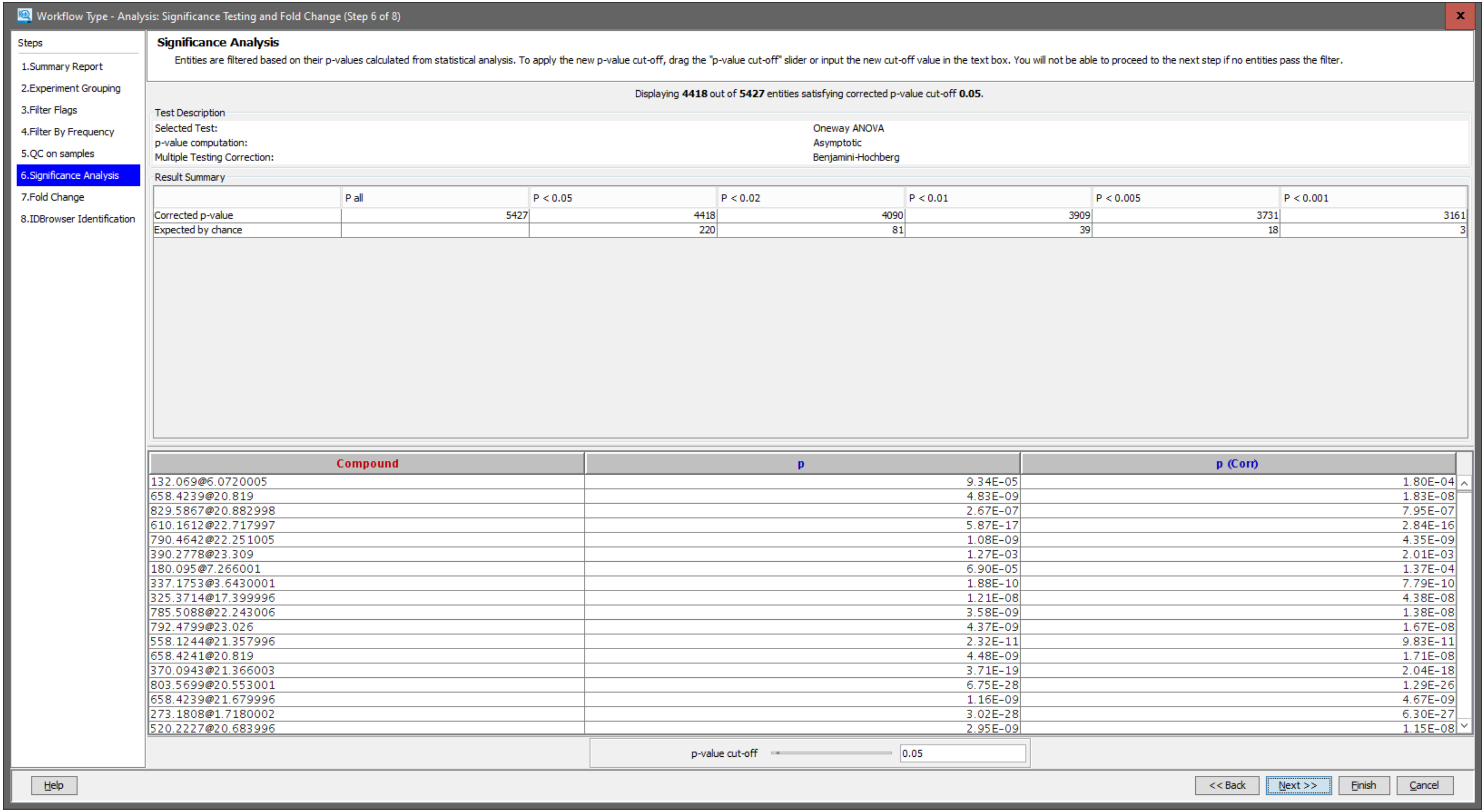
Legend - 3D PCA Scores

Color by Phaeodactylum.t

- 🟥 Media
- 🟨 J0-J1
- 🟦 J4
- 🟫 J5
- 🟩 J6
- 🟧 J8
- 🟦 Jmax10-11
- 🟥 Blank

Description
Algorithm: Principal Components Analysis
Parameters:
Column indices = [1-27]
Pruning option = [numPrincipalComponents, [4]]
Mean centered = true
Scale = true
3-D scores = true
PCA on = Columns

Suite message Justine nvel analysis: significance testing & Fold Change



Workflow Type - Analysis: Significance Testing and Fold Change (Step 6 of 8)

Significance Analysis

Entities are filtered based on their p-values calculated from statistical analysis. To apply the new p-value cut-off, drag the "p-value cut-off" slider or input the new cut-off value in the text box. You will not be able to proceed to the next step if no entities pass the filter.

Displaying **4418** out of **5427** entities satisfying corrected p-value cut-off **0.05.**

Test Description

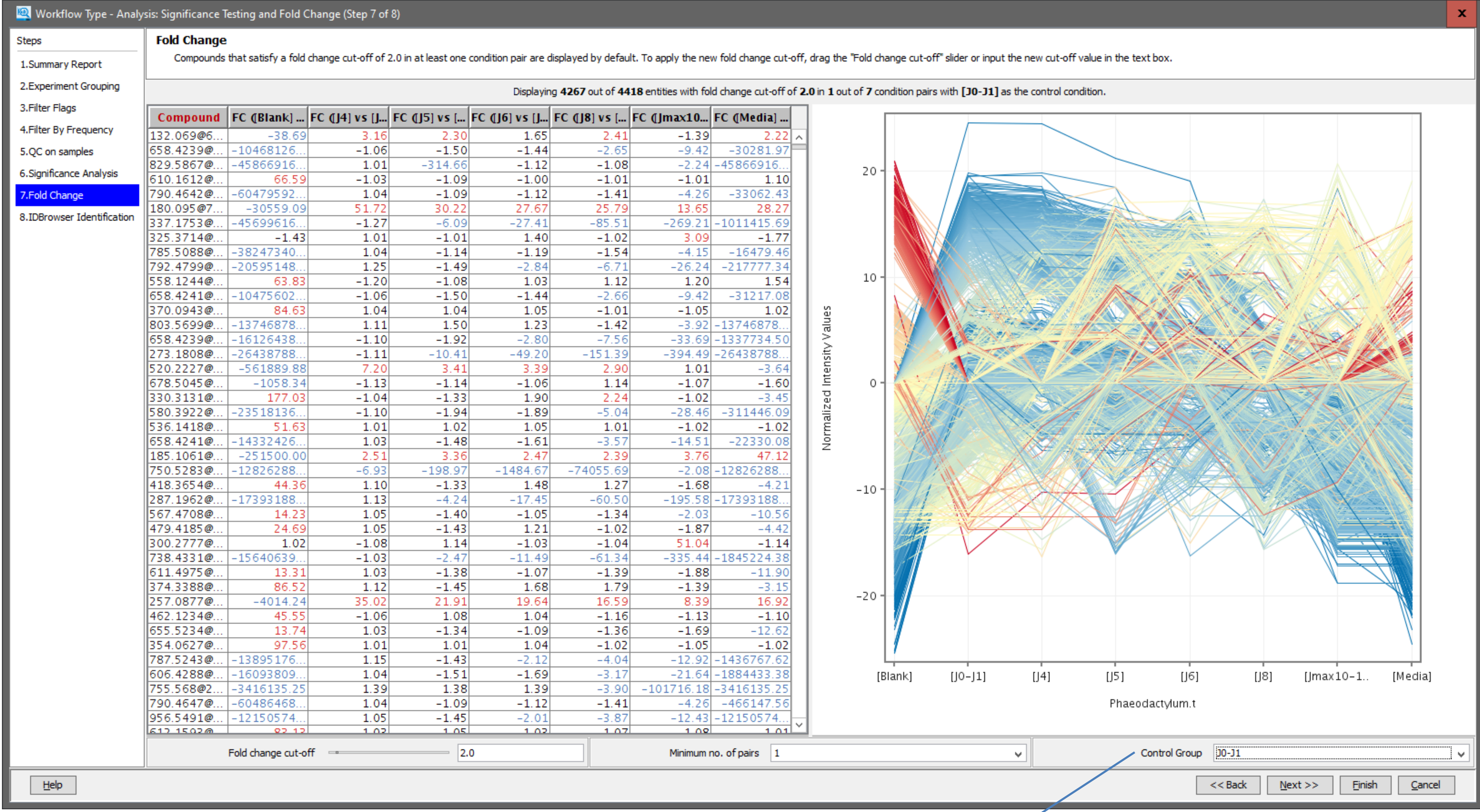
Selected Test:	Oneway ANOVA
p-value computation:	Asymptotic
Multiple Testing Correction:	Benjamini-Hochberg

Result Summary

	P all	P < 0.05	P < 0.02	P < 0.01	P < 0.005	P < 0.001
Corrected p-value	5427	4418	4090	3909	3731	3161
Expected by chance		220	81	39	18	3

Compound	p	p (Corr)
132.069@6.0720005	9.34E-05	1.80E-04
658.4239@20.819	4.83E-09	1.83E-08
829.5867@20.882998	2.67E-07	7.95E-07
610.1612@22.717997	5.87E-17	2.84E-16
790.4642@22.251005	1.08E-09	4.35E-09
390.2778@23.309	1.27E-03	2.01E-03
180.095@7.266001	6.90E-05	1.37E-04
337.1753@3.6430001	1.88E-10	7.79E-10
325.3714@17.399996	1.21E-08	4.38E-08
785.5088@22.243006	3.58E-09	1.38E-08
792.4799@23.026	4.37E-09	1.67E-08
558.1244@21.357996	2.32E-11	9.83E-11
658.4241@20.819	4.48E-09	1.71E-08
370.0943@21.366003	3.71E-19	2.04E-18
803.5699@20.553001	6.75E-28	1.29E-26
658.4239@21.679996	1.16E-09	4.67E-09
273.1808@1.7180002	3.02E-28	6.30E-27
520.2227@20.683996	2.95E-09	1.15E-08

p-value cut-off: 0.05



Fold Change

Compounds that satisfy a fold change cut-off of 2.0 in at least one condition pair are displayed by default. To apply the new fold change cut-off, drag the "Fold change cut-off" slider or input the new cut-off value in the text box.

Displaying **4267** out of **4418** entities with fold change cut-off of **2.0** in **1** out of **7** condition pairs with **[J0-J1]** as the control condition.

Compound	FC ([Blank] ...	FC ([J4] vs [J...	FC ([J5] vs [...	FC ([J6] vs [J...	FC ([J8] vs [...	FC ([Jmax10...	FC ([Media] ...
132.069@6...	-38.69	3.16	2.30	1.65	2.41	-1.39	2.22
658.4239@...	-10468126...	-1.06	-1.50	-1.44	-2.65	-9.42	-30281.97
829.5867@...	-45866916...	1.01	-314.66	-1.12	-1.08	-2.24	-45866916...
610.1612@...	66.59	-1.03	-1.09	-1.00	-1.01	-1.01	1.10
790.4642@...	-60479592...	1.04	-1.09	-1.12	-1.41	-4.26	-33062.43
180.095@7...	-30559.09	51.72	30.22	27.67	25.79	13.65	28.27
337.1753@...	-45699616...	-1.27	-6.09	-27.41	-85.51	-269.21	-1011415.69
325.3714@...	-1.43	1.01	-1.01	1.40	-1.02	3.09	-1.77
785.5088@...	-38247340...	1.04	-1.14	-1.19	-1.54	-4.15	-16479.46
792.4799@...	-20595148...	1.25	-1.49	-2.84	-6.71	-26.24	-217777.34
558.1244@...	63.83	-1.20	-1.08	1.03	1.12	1.20	1.54
658.4241@...	-10475602...	-1.06	-1.50	-1.44	-2.66	-9.42	-31217.08
370.0943@...	84.63	1.04	1.04	1.05	-1.01	-1.05	1.02
803.5699@...	-13746878...	1.11	1.50	1.23	-1.42	-3.92	-13746878...
658.4239@...	-16126438...	-1.10	-1.92	-2.80	-7.56	-33.69	-1337734.50
273.1808@...	-26438788...	-1.11	-10.41	-49.20	-151.39	-394.49	-26438788...
520.2227@...	-561889.88	7.20	3.41	3.39	2.90	1.01	-3.64
678.5045@...	-1058.34	-1.13	-1.14	-1.06	1.14	-1.07	-1.60
330.3131@...	177.03	-1.04	-1.33	1.90	2.24	-1.02	-3.45
580.3922@...	-23518136...	-1.10	-1.94	-1.89	-5.04	-28.46	-311446.09
536.1418@...	51.63	1.01	1.02	1.05	1.01	-1.02	-1.02
658.4241@...	-14332426...	1.03	-1.48	-1.61	-3.57	-14.51	-22330.08
185.1061@...	-251500.00	2.51	3.36	2.47	2.39	3.76	47.12
750.5283@...	-12826288...	-6.93	-198.97	-1484.67	-74055.69	-2.08	-12826288...
418.3654@...	44.36	1.10	-1.33	1.48	1.27	-1.68	-4.21
287.1962@...	-17393188...	1.13	-4.24	-17.45	-60.50	-195.58	-17393188...
567.4708@...	14.23	1.05	-1.40	-1.05	-1.34	-2.03	-10.56
479.4185@...	24.69	1.05	-1.43	1.21	-1.02	-1.87	-4.42
300.2777@...	1.02	-1.08	1.14	-1.03	-1.04	51.04	-1.14
738.4331@...	-15640639...	-1.03	-2.47	-11.49	-61.34	-335.44	-1845224.38
611.4975@...	13.31	1.03	-1.38	-1.07	-1.39	-1.88	-11.90
374.3388@...	86.52	1.12	-1.45	1.68	1.79	-1.39	-3.15
257.0877@...	-4014.24	35.02	21.91	19.64	16.59	8.39	16.92
462.1234@...	45.55	-1.06	1.08	1.04	-1.16	-1.13	-1.10
655.5234@...	13.74	1.03	-1.34	-1.09	-1.36	-1.69	-12.62
354.0627@...	97.56	1.01	1.01	1.04	-1.02	-1.05	-1.02
787.5243@...	-13895176...	1.15	-1.43	-2.12	-4.04	-12.92	-1436767.62
606.4288@...	-16093809...	1.04	-1.51	-1.69	-3.17	-21.64	-1884433.38
755.568@2...	-3416135.25	1.39	1.38	1.39	-3.90	-101716.18	-3416135.25
790.4647@...	-60486468...	1.04	-1.09	-1.12	-1.41	-4.26	-466147.56
956.5491@...	-12150574...	1.05	-1.45	-2.01	-3.87	-12.43	-12150574...

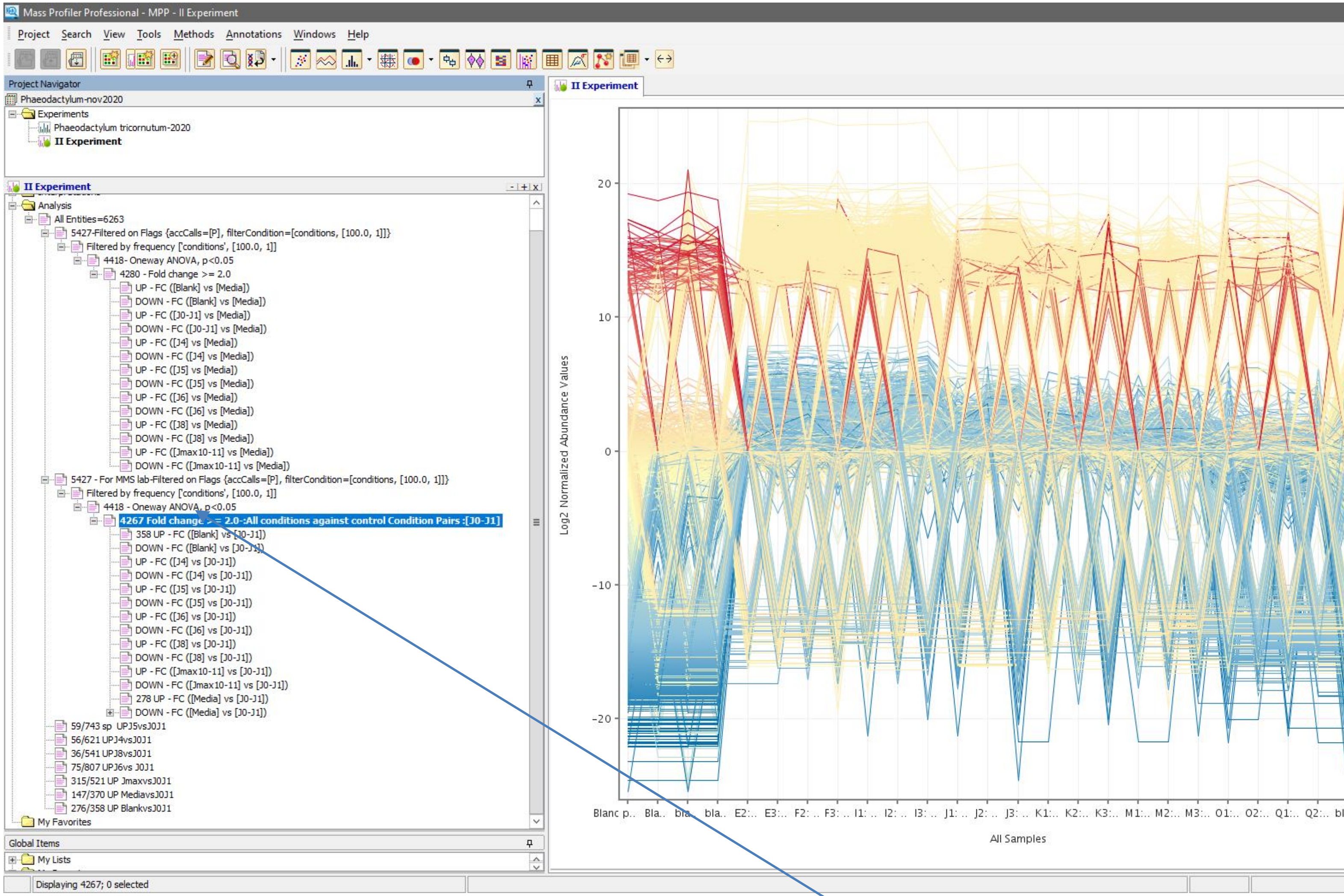
Fold change cut-off: 2.0

Minimum no. of pairs: 1

Control Group: J0-J1

Changement de groupe et J0-J1 sert de contrôle

6- 2020 New Phaeodactylum MPP15v1.tar



- Phaeodactylum-nov2020
  - Experiments
    - Phaeodactylum tricornutum-2020
    - **II Experiment**

II Experiment

- Analysis
  - All Entities=6263
    - 5427-Filtered on Flags {accCalls=[P], filterCondition=[conditions, [100.0, 1]]}
      - Filtered by frequency ['conditions', [100.0, 1]]
        - 4418- Oneway ANOVA, p<0.05
          - 4280 - Fold change >= 2.0
            - UP - FC ([Blank] vs [Media])
            - DOWN - FC ([Blank] vs [Media])
            - UP - FC ([J0-J1] vs [Media])
            - DOWN - FC ([J0-J1] vs [Media])
            - UP - FC ([J4] vs [Media])
            - DOWN - FC ([J4] vs [Media])
            - UP - FC ([J5] vs [Media])
            - DOWN - FC ([J5] vs [Media])
            - UP - FC ([J6] vs [Media])
            - DOWN - FC ([J6] vs [Media])
            - UP - FC ([J8] vs [Media])
            - DOWN - FC ([J8] vs [Media])
            - UP - FC ([Jmax10-11] vs [Media])
            - DOWN - FC ([Jmax10-11] vs [Media])
    - 5427 - For MMS lab-Filtered on Flags {accCalls=[P], filterCondition=[conditions, [100.0, 1]]}
      - Filtered by frequency ['conditions', [100.0, 1]]
        - 4418 - Oneway ANOVA, p<0.05
          - 4267 Fold change >= 2.0-:All conditions against control Condition Pairs :[J0-J1]
            - 358 UP - FC ([Blank] vs [J0-J1])
            - DOWN - FC ([Blank] vs [J0-J1])
            - UP - FC ([J4] vs [J0-J1])
            - DOWN - FC ([J4] vs [J0-J1])
            - UP - FC ([J5] vs [J0-J1])
            - DOWN - FC ([J5] vs [J0-J1])
            - UP - FC ([J6] vs [J0-J1])
            - DOWN - FC ([J6] vs [J0-J1])
            - UP - FC ([J8] vs [J0-J1])
            - DOWN - FC ([J8] vs [J0-J1])
            - UP - FC ([Jmax10-11] vs [J0-J1])
            - DOWN - FC ([Jmax10-11] vs [J0-J1])
            - 278 UP - FC ([Media] vs [J0-J1])
            - DOWN - FC ([Media] vs [J0-J1])
    - 59/743 sp UPJ5vsJ0J1
    - 56/621 UPJ4vsJ0J1
    - 36/541 UPJ8vsJ0J1
    - 75/807 UPJ6vs J0J1
    - 315/521 UP JmaxvsJ0J1
    - 147/370 UP MediavsJ0J1
    - 276/358 UP BlankvsJ0J1
- My Favorites

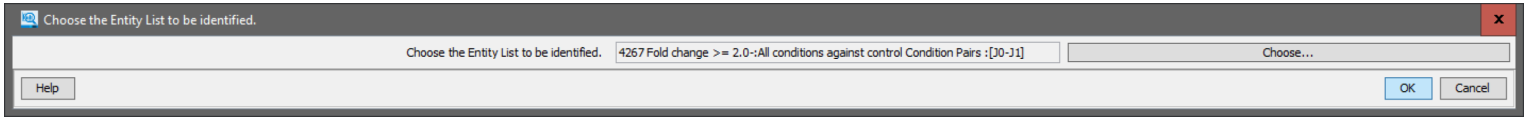
Global Items

- My Lists

Displaying 4267; 0 selected

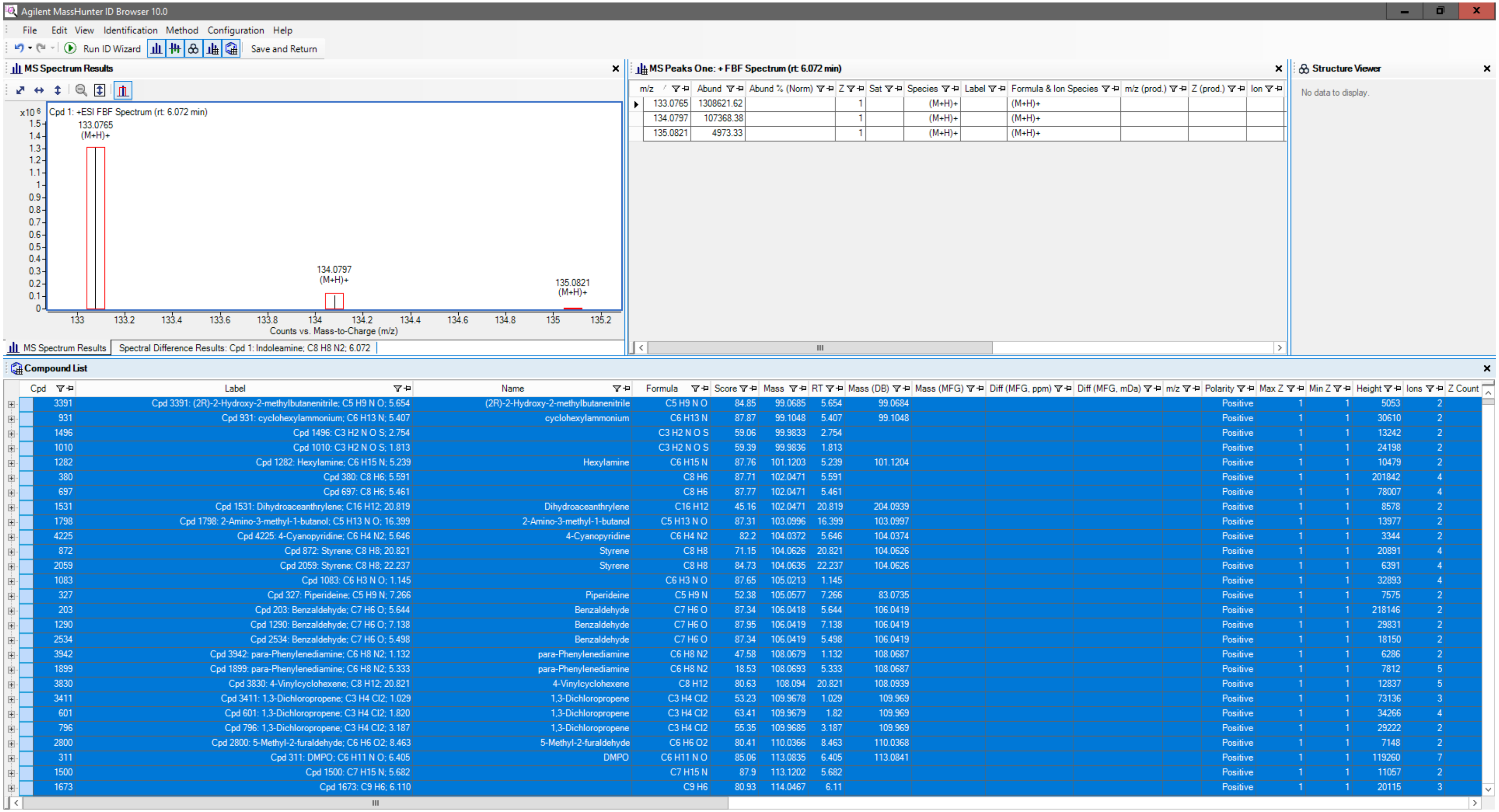
Extraction du fichier : Phaeodactylum (without E1-F1) Foldchange sur J0-J1controle.xlsx 4267 entities comparés à la transcriptomique sur 115 composés communs (Results on115 composés MMS rev FM.xlsx)

Results interprétation by IDBrowser Identification



Choose the Entity List to be identified.

Choose the Entity List to be identified. 4267 Fold change >= 2.0-:All conditions against control Condition Pairs :[J0-J1]



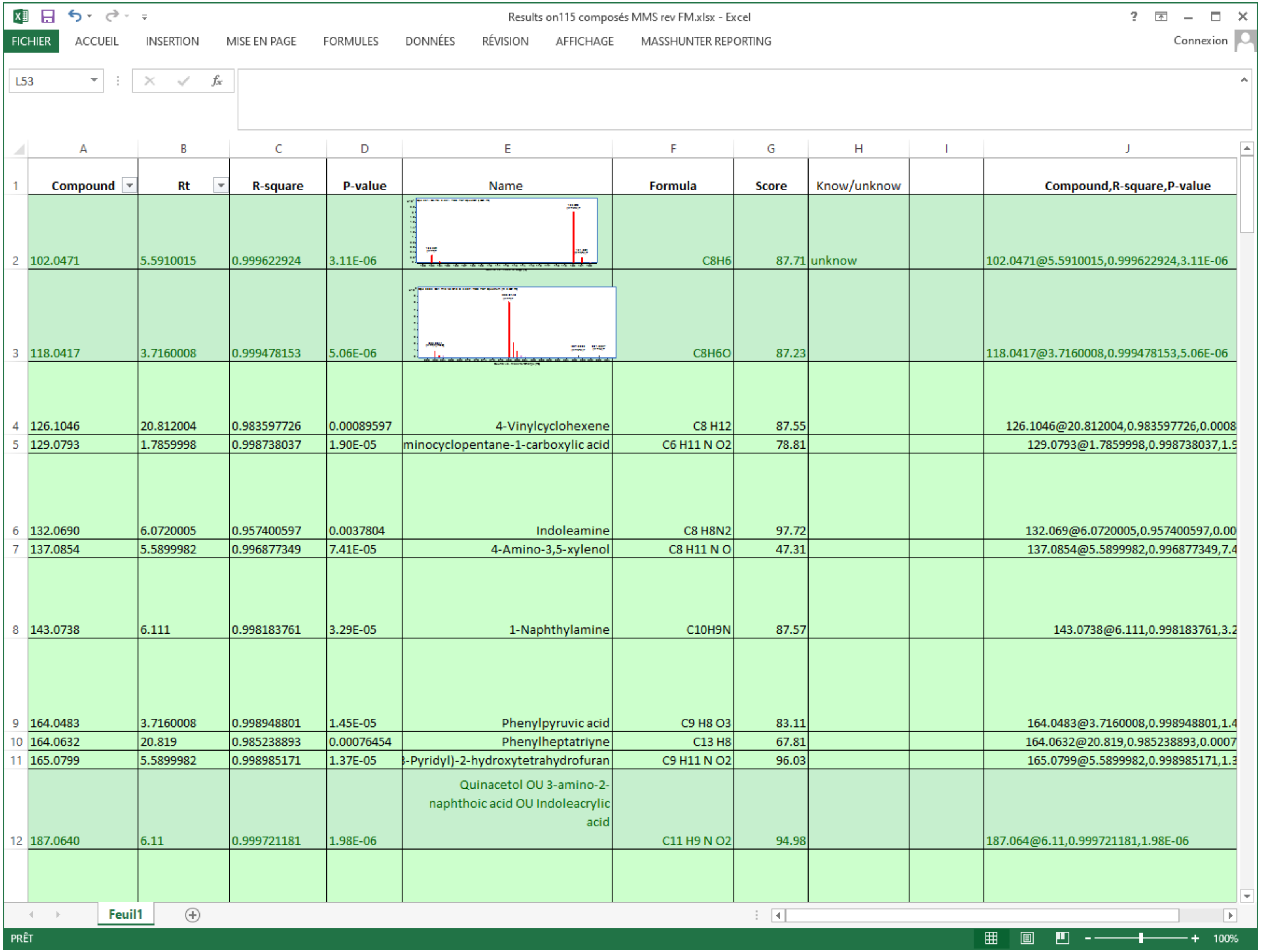
MS Peaks One: + FBF Spectrum (rt: 6.072 min)

m/z	Abund	Abund % (Norm)	Z	Sat	Species	Label	Formula & Ion Species	m/z (prod.)	Z (prod.)	Ion
133.0765	1308621.62		1		(M+H)+		(M+H)+			
134.0797	107368.38		1		(M+H)+		(M+H)+			
135.0821	4973.33		1		(M+H)+		(M+H)+			

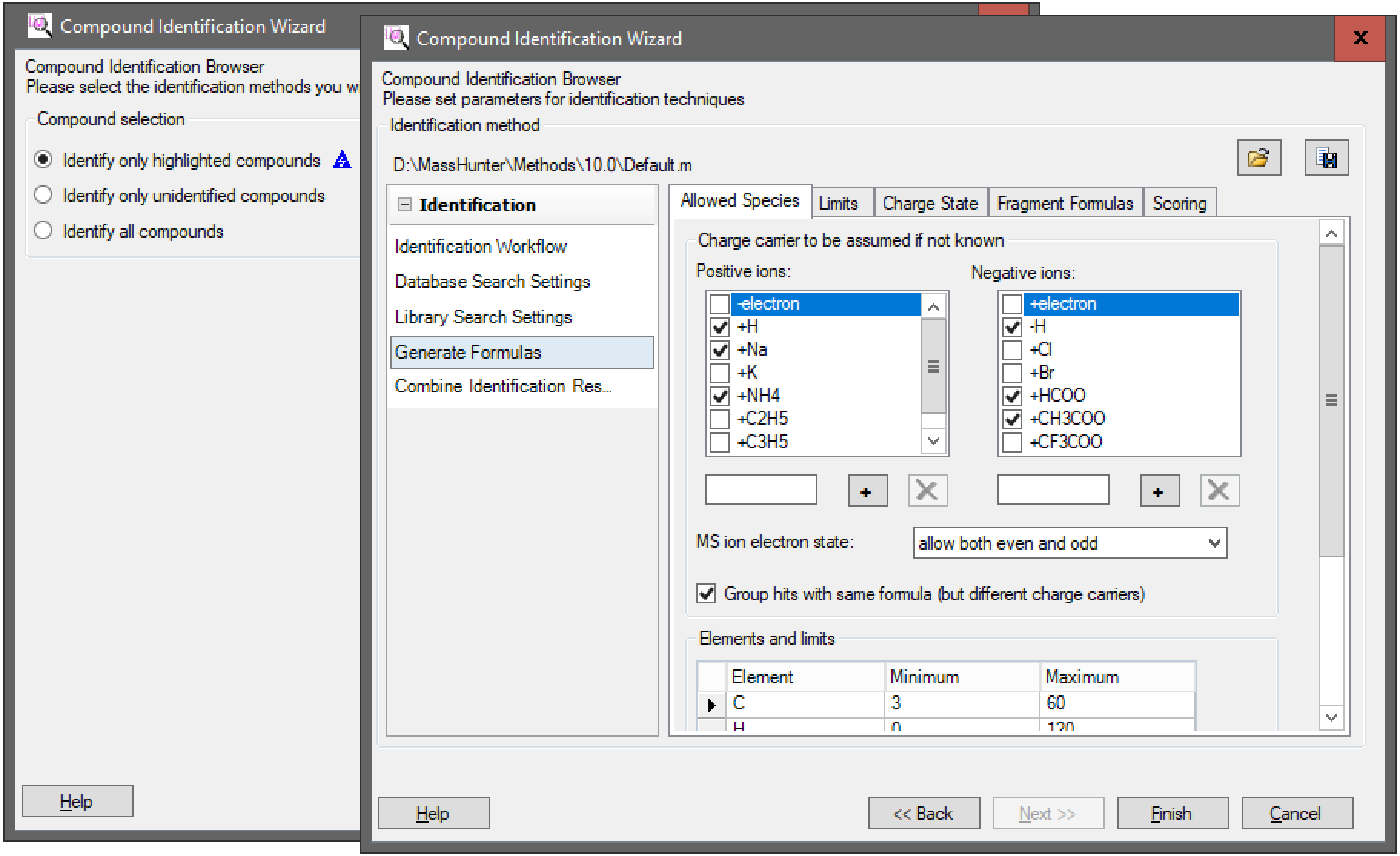
Compound List

Cpd	Label	Name	Formula	Score	Mass	RT	Mass (DB)	Mass (MFG)	Diff (MFG, ppm)	Diff (MFG, mDa)	m/z	Polarity	Max Z	Min Z	Height	Ions	Z Count
3391	Cpd 3391: (2R)-2-Hydroxy-2-methylbutanenitrile; C5 H9 N O; 5.654	(2R)-2-Hydroxy-2-methylbutanenitrile	C5 H9 N O	84.85	99.0685	5.654	99.0684					Positive	1	1	5053	2	
931	Cpd 931: cyclohexylammonium; C6 H13 N; 5.407	cyclohexylammonium	C6 H13 N	87.87	99.1048	5.407	99.1048					Positive	1	1	30610	2	
1496	Cpd 1496: C3 H2 N O S; 2.754		C3 H2 N O S	59.06	99.9833	2.754						Positive	1	1	13242	2	
1010	Cpd 1010: C3 H2 N O S; 1.813		C3 H2 N O S	59.39	99.9836	1.813						Positive	1	1	24198	2	
1282	Cpd 1282: Hexylamine; C6 H15 N; 5.239	Hexylamine	C6 H15 N	87.76	101.1203	5.239	101.1204					Positive	1	1	10479	2	
380	Cpd 380: C8 H6; 5.591		C8 H6	87.71	102.0471	5.591						Positive	1	1	201842	4	
697	Cpd 697: C8 H6; 5.461		C8 H6	87.77	102.0471	5.461						Positive	1	1	78007	4	
1531	Cpd 1531: Dihydroaceanthrylene; C16 H12; 20.819	Dihydroaceanthrylene	C16 H12	45.16	102.0471	20.819	204.0939					Positive	1	1	8578	2	
1798	Cpd 1798: 2-Amino-3-methyl-1-butanol; C5 H13 N O; 16.399	2-Amino-3-methyl-1-butanol	C5 H13 N O	87.31	103.0996	16.399	103.0997					Positive	1	1	13977	2	
4225	Cpd 4225: 4-Cyanopyridine; C6 H4 N2; 5.646	4-Cyanopyridine	C6 H4 N2	82.2	104.0372	5.646	104.0374					Positive	1	1	3344	2	
872	Cpd 872: Styrene; C8 H8; 20.821	Styrene	C8 H8	71.15	104.0626	20.821	104.0626					Positive	1	1	20891	4	
2059	Cpd 2059: Styrene; C8 H8; 22.237	Styrene	C8 H8	84.73	104.0635	22.237	104.0626					Positive	1	1	6391	4	
1083	Cpd 1083: C6 H3 N O; 1.145		C6 H3 N O	87.65	105.0213	1.145						Positive	1	1	32893	4	
327	Cpd 327: Piperideine; C5 H9 N; 7.266	Piperideine	C5 H9 N	52.38	105.0577	7.266	83.0735					Positive	1	1	7575	2	
203	Cpd 203: Benzaldehyde; C7 H6 O; 5.644	Benzaldehyde	C7 H6 O	87.34	106.0418	5.644	106.0419					Positive	1	1	218146	2	
1290	Cpd 1290: Benzaldehyde; C7 H6 O; 7.138	Benzaldehyde	C7 H6 O	87.95	106.0419	7.138	106.0419					Positive	1	1	29831	2	
2534	Cpd 2534: Benzaldehyde; C7 H6 O; 5.498	Benzaldehyde	C7 H6 O	87.34	106.0419	5.498	106.0419					Positive	1	1	18150	2	
3942	Cpd 3942: para-Phenylenediamine; C6 H8 N2; 1.132	para-Phenylenediamine	C6 H8 N2	47.58	108.0679	1.132	108.0687					Positive	1	1	6286	2	
1899	Cpd 1899: para-Phenylenediamine; C6 H8 N2; 5.333	para-Phenylenediamine	C6 H8 N2	18.53	108.0693	5.333	108.0687					Positive	1	1	7812	5	
3830	Cpd 3830: 4-Vinylcyclohexene; C8 H12; 20.821	4-Vinylcyclohexene	C8 H12	80.63	108.094	20.821	108.0939					Positive	1	1	12837	5	
3411	Cpd 3411: 1,3-Dichloropropene; C3 H4 Cl2; 1.029	1,3-Dichloropropene	C3 H4 Cl2	53.23	109.9678	1.029	109.969					Positive	1	1	73136	3	
601	Cpd 601: 1,3-Dichloropropene; C3 H4 Cl2; 1.820	1,3-Dichloropropene	C3 H4 Cl2	63.41	109.9679	1.82	109.969					Positive	1	1	34266	4	
796	Cpd 796: 1,3-Dichloropropene; C3 H4 Cl2; 3.187	1,3-Dichloropropene	C3 H4 Cl2	55.35	109.9685	3.187	109.969					Positive	1	1	29222	2	
2800	Cpd 2800: 5-Methyl-2-furaldehyde; C6 H6 O2; 8.463	5-Methyl-2-furaldehyde	C6 H6 O2	80.41	110.0366	8.463	110.0368					Positive	1	1	7148	2	
311	Cpd 311: DMPO; C6 H11 N O; 6.405	DMPO	C6 H11 N O	85.06	113.0835	6.405	113.0841					Positive	1	1	119260	7	
1500	Cpd 1500: C7 H15 N; 5.682		C7 H15 N	87.9	113.1202	5.682						Positive	1	1	11057	2	
1673	Cpd 1673: C9 H6; 6.110		C9 H6	80.93	114.0467	6.11						Positive	1	1	20115	3	

Pour compléter l'identification des composés commun à la transcriptomique



	A	B	C	D	E	F	G	H	I	J
1	**Compound**	**Rt**	**R-square**	**P-value**	Name	**Formula**	**Score**	Know/unknow		**Compound,R-square,P-value**
2	102.0471	5.5910015	0.999622924	3.11E-06		C8H6	87.71	unknow		102.0471@5.5910015,0.999622924,3.11E-06
3	118.0417	3.7160008	0.999478153	5.06E-06		C8H6O	87.23			118.0417@3.7160008,0.999478153,5.06E-06
4	126.1046	20.812004	0.983597726	0.00089597	4-Vinylcyclohexene	C8 H12	87.55			126.1046@20.812004,0.983597726,0.0008
5	129.0793	1.7859998	0.998738037	1.90E-05	minocyclopentane-1-carboxylic acid	C6 H11 N O2	78.81			129.0793@1.7859998,0.998738037,1.9
6	132.0690	6.0720005	0.957400597	0.0037804	Indoleamine	C8 H8N2	97.72			132.069@6.0720005,0.957400597,0.00
7	137.0854	5.5899982	0.996877349	7.41E-05	4-Amino-3,5-xylenol	C8 H11 N O	47.31			137.0854@5.5899982,0.996877349,7.4
8	143.0738	6.111	0.998183761	3.29E-05	1-Naphthylamine	C10H9N	87.57			143.0738@6.111,0.998183761,3.2
9	164.0483	3.7160008	0.998948801	1.45E-05	Phenylpyruvic acid	C9 H8 O3	83.11			164.0483@3.7160008,0.998948801,1.4
10	164.0632	20.819	0.985238893	0.00076454	Phenylheptatriyne	C13 H8	67.81			164.0632@20.819,0.985238893,0.0007
11	165.0799	5.5899982	0.998985171	1.37E-05	-Pyridyl)-2-hydroxytetrahydrofuran	C9 H11 N O2	96.03			165.0799@5.5899982,0.998985171,1.3
12	187.0640	6.11	0.999721181	1.98E-06	Quinacetol OU 3-amino-2-naphthoic acid OU Indoleacrylic acid	C11 H9 N O2	94.98			187.064@6.11,0.999721181,1.98E-06



Compound Identification Browser
Please select the identification methods you w

Compound selection

● Identify only highlighted compounds
○ Identify only unidentified compounds
○ Identify all compounds

Compound Identification Browser
Please set parameters for identification techniques

Identification method

D:\MassHunter\Methods\10.0\Default.m

Identification
- Identification Workflow
- Database Search Settings
- Library Search Settings
- Generate Formulas
- Combine Identification Res...

Charge carrier to be assumed if not known

Positive ions:
- ☐ -electron
- ☑ +H
- ☑ +Na
- ☐ +K
- ☑ +NH4
- ☐ +C2H5
- ☐ +C3H5

Negative ions:
- ☐ +electron
- ☑ -H
- ☐ +Cl
- ☐ +Br
- ☑ +HCOO
- ☑ +CH3COO
- ☐ +CF3COO

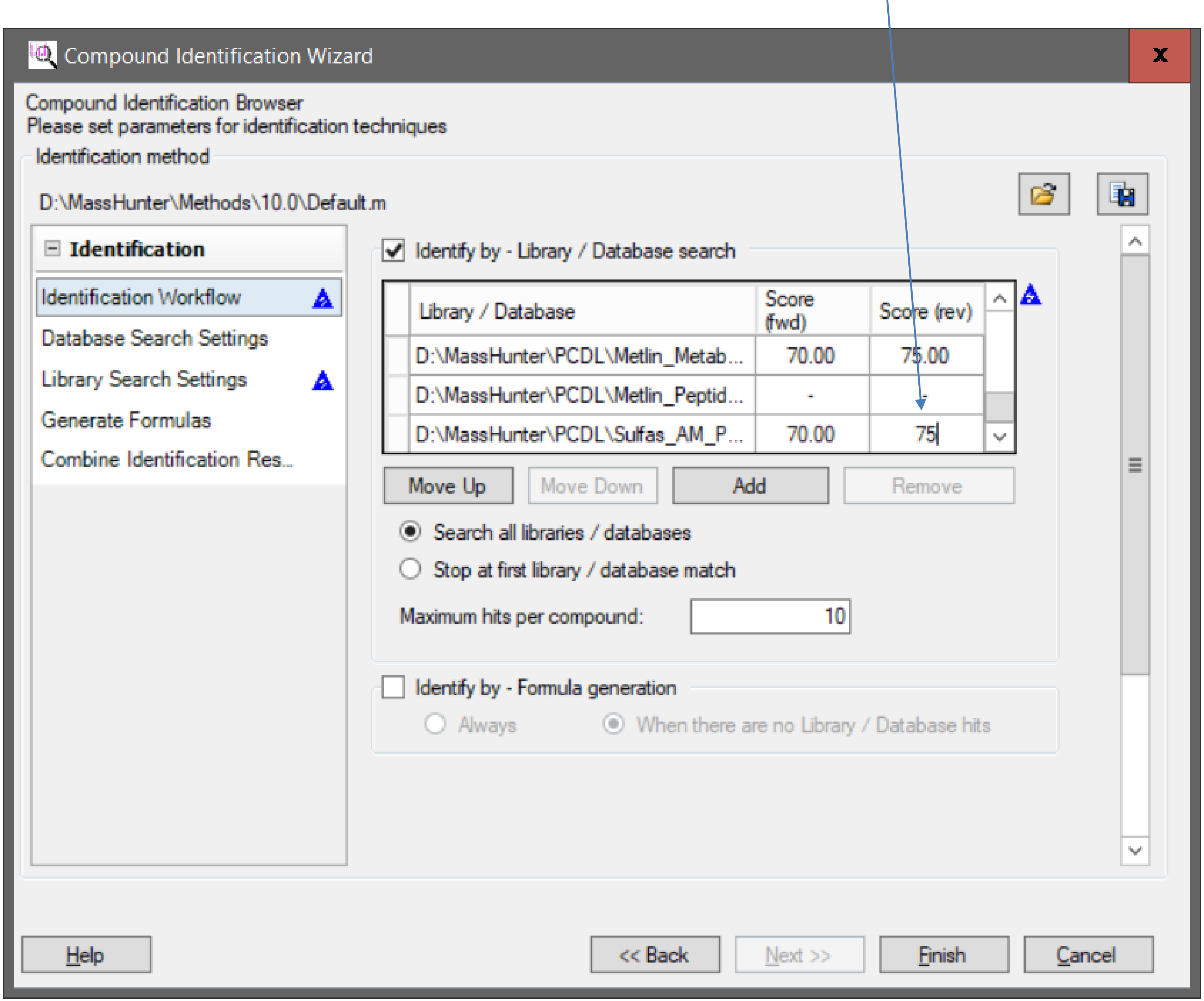
MS ion electron state: allow both even and odd

☑ Group hits with same formula (but different charge carriers)

Elements and limits

Element	Minimum	Maximum
C	3	60
H	0	120

Il faudrait recommencer l'analyse sur l'ensemble des base en spécifiant le nb de C, H, N, etc de telle manière que l'on n'ait pas de N14 (max5) et augmenter le nb de C pour ne pas etre sous la lim… bref de manière à améliorer le score des 115 composés à identifier à faire: 04/02/2021



Compound Identification Wizard

Compound Identification Browser
Please set parameters for identification techniques

Identification method

D:\MassHunter\Methods\10.0\Default.m

Identification

- Identification Workflow
- Database Search Settings
- Library Search Settings
- Generate Formulas
- Combine Identification Res...

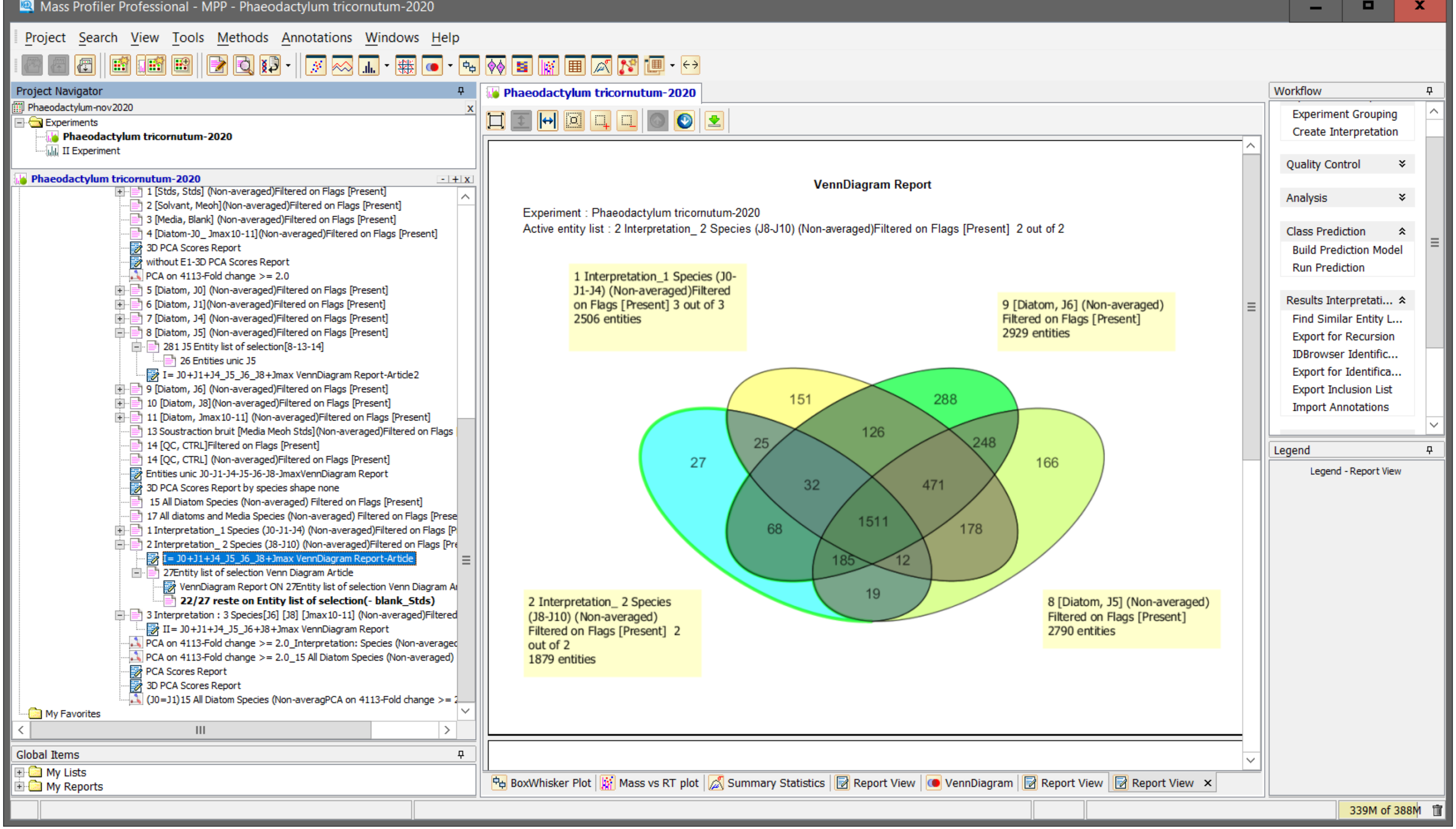
☑ Identify by - Library / Database search

Library / Database	Score (fwd)	Score (rev)
D:\MassHunter\PCDL\Metlin_Metab...	70.00	75.00
D:\MassHunter\PCDL\Metlin_Peptid...	-	-
D:\MassHunter\PCDL\Sulfas_AM_P...	70.00	75

● Search all libraries / databases
○ Stop at first library / database match

Maximum hits per compound: 10

☐ Identify by - Formula generation
○ Always ● When there are no Library / Database hits



VennDiagram Report

Experiment : Phaeodactylum tricornutum-2020
Active entity list : 2 Interpretation_ 2 Species (J8-J10) (Non-averaged)Filtered on Flags [Present] 2 out of 2

1 Interpretation_1 Species (J0-J1-J4) (Non-averaged)Filtered on Flags [Present] 3 out of 3
2506 entities

9 [Diatom, J6] (Non-averaged) Filtered on Flags [Present]
2929 entities

2 Interpretation_ 2 Species (J8-J10) (Non-averaged) Filtered on Flags [Present] 2 out of 2
1879 entities

8 [Diatom, J5] (Non-averaged) Filtered on Flags [Present]
2790 entities

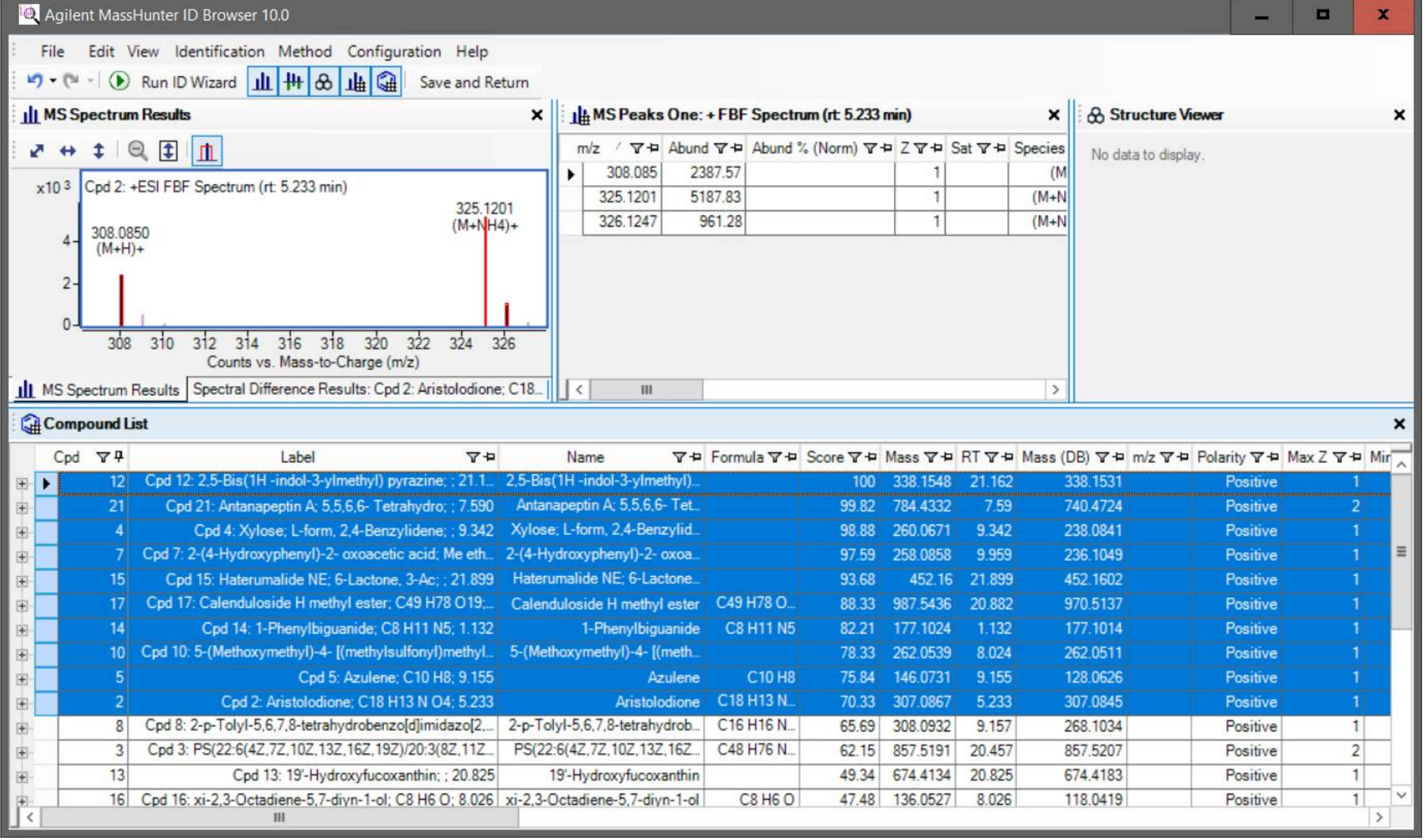
Comparaison Analyse 1:

Hy1= J0+JJ+J4; - J5; - J6 et Hy2= J8+Jmax

Avec Hy1 100% of the values in any 3 out of 3 conditions have acceptable values

Et Hy2 2 out of 2

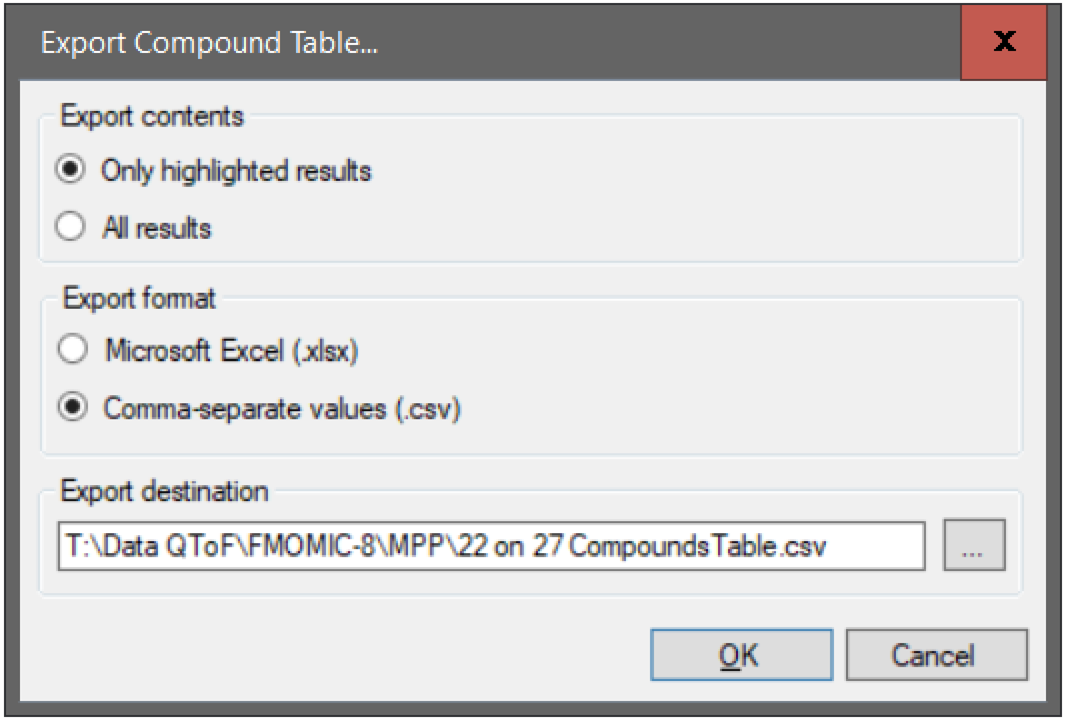
puis Results interprétation by IDBrowser Identification sur le compartiment 27 (Demandé par Justine)



m/z	Abund	Abund % (Norm)	Z	Sat	Species
308.085	2387.57		1		(M
325.1201	5187.83		1		(M+N
326.1247	961.28		1		(M+N

Cpd	Label	Name	Formula	Score	Mass	RT	Mass (DB)	m/z	Polarity	Max Z	Mir
12	Cpd 12: 2,5-Bis(1H -indol-3-ylmethyl) pyrazine; ; 21.1...	2,5-Bis(1H -indol-3-ylmethyl)...		100	338.1548	21.162	338.1531		Positive	1	
21	Cpd 21: Antanapeptin A; 5,5,6,6- Tetrahydro; ; 7.590	Antanapeptin A; 5,5,6,6- Tet...		99.82	784.4332	7.59	740.4724		Positive	2	
4	Cpd 4: Xylose; L-form, 2,4-Benzylidene; ; 9.342	Xylose; L-form, 2,4-Benzylid...		98.88	260.0671	9.342	238.0841		Positive	1	
7	Cpd 7: 2-(4-Hydroxyphenyl)-2- oxoacetic acid; Me eth...	2-(4-Hydroxyphenyl)-2- oxoa...		97.59	258.0858	9.959	236.1049		Positive	1	
15	Cpd 15: Haterumalide NE; 6-Lactone, 3-Ac; ; 21.899	Haterumalide NE; 6-Lactone...		93.68	452.16	21.899	452.1602		Positive	1	
17	Cpd 17: Calenduloside H methyl ester; C49 H78 O19;...	Calenduloside H methyl ester	C49 H78 O...	88.33	987.5436	20.882	970.5137		Positive	1	
14	Cpd 14: 1-Phenylbiguanide; C8 H11 N5; 1.132	1-Phenylbiguanide	C8 H11 N5	82.21	177.1024	1.132	177.1014		Positive	1	
10	Cpd 10: 5-(Methoxymethyl)-4- [(methylsulfonyl)methyl...	5-(Methoxymethyl)-4- [(meth...		78.33	262.0539	8.024	262.0511		Positive	1	
5	Cpd 5: Azulene; C10 H8; 9.155	Azulene	C10 H8	75.84	146.0731	9.155	128.0626		Positive	1	
2	Cpd 2: Aristolodione; C18 H13 N O4; 5.233	Aristolodione	C18 H13 N...	70.33	307.0867	5.233	307.0845		Positive	1	
8	Cpd 8: 2-p-Tolyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,...	2-p-Tolyl-5,6,7,8-tetrahydrob...	C16 H16 N...	65.69	308.0932	9.157	268.1034		Positive	1	
3	Cpd 3: PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:3(8Z,11Z...	PS(22:6(4Z,7Z,10Z,13Z,16Z...	C48 H76 N...	62.15	857.5191	20.457	857.5207		Positive	2	
13	Cpd 13: 19'-Hydroxyfucoxanthin; ; 20.825	19'-Hydroxyfucoxanthin		49.34	674.4134	20.825	674.4183		Positive	1	
16	Cpd 16: xi-2,3-Octadiene-5,7-diyn-1-ol; C8 H6 O; 8.026	xi-2,3-Octadiene-5,7-diyn-1-ol	C8 H6 O	47.48	136.0527	8.026	118.0419		Positive	1	

File-Export compound table

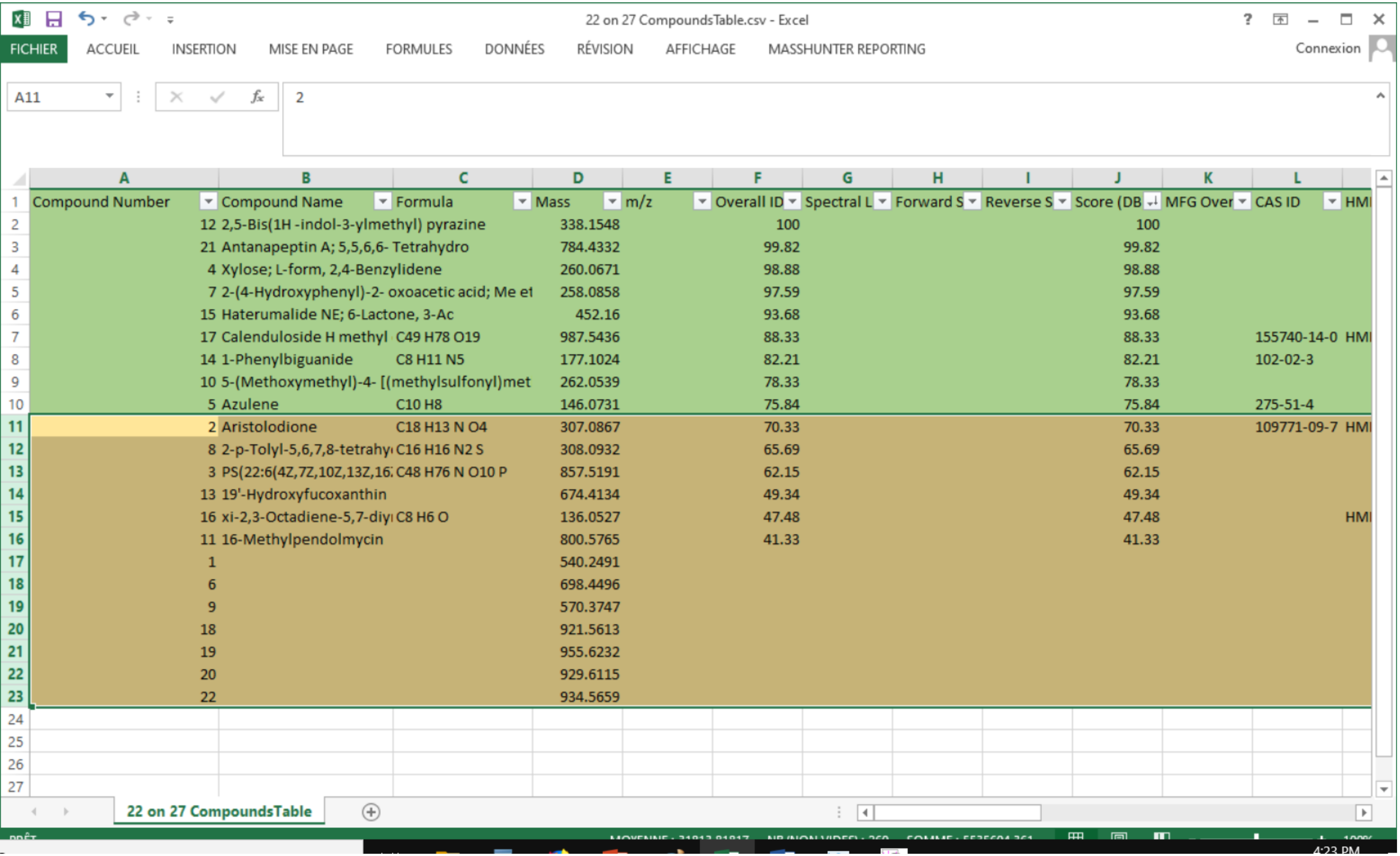


Export contents
● Only highlighted results
○ All results

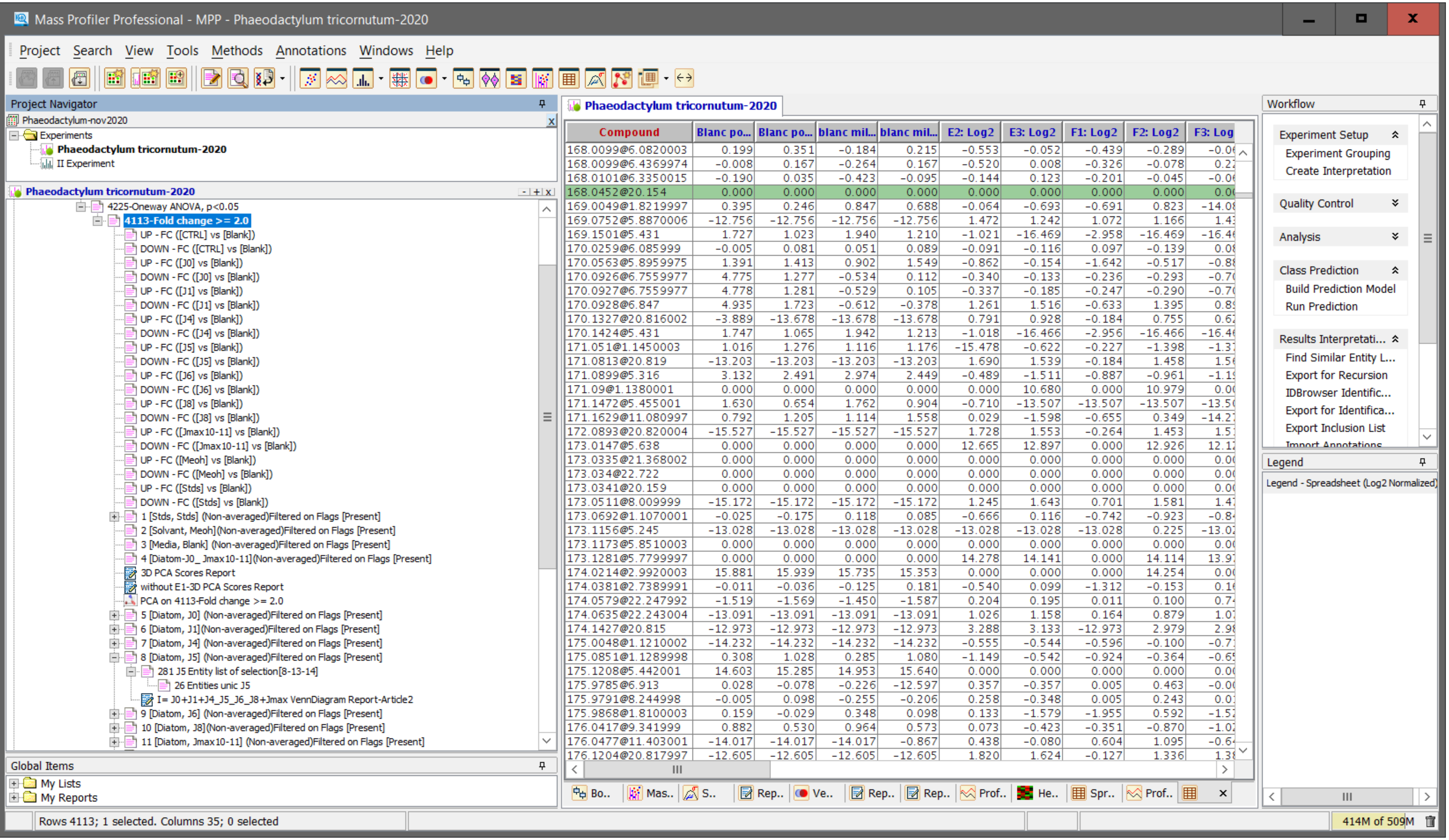
Export format
○ Microsoft Excel (.xlsx)
● Comma-separate values (.csv)

Export destination
T:\Data QToF\FMOMIC-8\MPP\22 on 27 CompoundsTable.csv

Ouvrir ce fichier. Csv dans Excel (séparateur: point-virgule)
Recherche du phosphoenolpyruvate; Phosphoenolpyruvic acid; 138-08-9; 2-Propenoic acid, 2-(phosphonooxy)-; 2-(phosphonooxy)prop-2-enoic acid; Phosphopyruvic acid; 2-Phosphonooxyprop-2-enoic acid; PEP; ...
Compound CID: 1005
MF: $C_3H_5O_6P$
MW: 168.04g/mol
InChIKey: DTBNBXWJWCWCIK-UHFFFAOYSA-N
IUPAC Name: 2-phosphonooxyprop-2-enoic acid
Create Date: 2004-09-16



	A	B	C	D	E	F	G	H	I	J	K	L	
1	Compound Number	Compound Name	Formula	Mass	m/z	Overall ID	Spectral L	Forward S	Reverse S	Score (DB	MFG Over	CAS ID	HMI
2	12	2,5-Bis(1H -indol-3-ylmethyl) pyrazine		338.1548		100				100			
3	21	Antanapeptin A; 5,5,6,6- Tetrahydro		784.4332		99.82				99.82			
4	4	Xylose; L-form, 2,4-Benzylidene		260.0671		98.88				98.88			
5	7	2-(4-Hydroxyphenyl)-2- oxoacetic acid; Me et		258.0858		97.59				97.59			
6	15	Haterumalide NE; 6-Lactone, 3-Ac		452.16		93.68				93.68			
7	17	Calenduloside H methyl	C49 H78 O19	987.5436		88.33				88.33		155740-14-0	HMI
8	14	1-Phenylbiguanide	C8 H11 N5	177.1024		82.21				82.21		102-02-3	
9	10	5-(Methoxymethyl)-4- [(methylsulfonyl)met		262.0539		78.33				78.33			
10	5	Azulene	C10 H8	146.0731		75.84				75.84		275-51-4	
11	2	Aristolodione	C18 H13 N O4	307.0867		70.33				70.33		109771-09-7	HMI
12	8	2-p-Tolyl-5,6,7,8-tetrahy	C16 H16 N2 S	308.0932		65.69				65.69			
13	3	PS(22:6(4Z,7Z,10Z,13Z,16	C48 H76 N O10 P	857.5191		62.15				62.15			
14	13	19'-Hydroxyfucoxanthin		674.4134		49.34				49.34			
15	16	xi-2,3-Octadiene-5,7-diy	C8 H6 O	136.0527		47.48				47.48			HMI
16	11	16-Methylpendolmycin		800.5765		41.33				41.33			
17	1			540.2491									
18	6			698.4496									
19	9			570.3747									
20	18			921.5613									
21	19			955.6232									
22	20			929.6115									
23	22			934.5659									
24													
25													
26													
27													



Phaeodactylum-nov2020
- Experiments
  - **Phaeodactylum tricornutum-2020**
  - II Experiment

Phaeodactylum tricornutum-2020
- 4225-Oneway ANOVA, p<0.05
  - 4113-Fold change >= 2.0
    - UP - FC ([CTRL] vs [Blank])
    - DOWN - FC ([CTRL] vs [Blank])
    - UP - FC ([J0] vs [Blank])
    - DOWN - FC ([J0] vs [Blank])
    - UP - FC ([J1] vs [Blank])
    - DOWN - FC ([J1] vs [Blank])
    - UP - FC ([J4] vs [Blank])
    - DOWN - FC ([J4] vs [Blank])
    - UP - FC ([J5] vs [Blank])
    - DOWN - FC ([J5] vs [Blank])
    - UP - FC ([J6] vs [Blank])
    - DOWN - FC ([J6] vs [Blank])
    - UP - FC ([J8] vs [Blank])
    - DOWN - FC ([J8] vs [Blank])
    - UP - FC ([Jmax10-11] vs [Blank])
    - DOWN - FC ([Jmax10-11] vs [Blank])
    - UP - FC ([Meoh] vs [Blank])
    - DOWN - FC ([Meoh] vs [Blank])
    - UP - FC ([Stds] vs [Blank])
    - DOWN - FC ([Stds] vs [Blank])
    - 1 [Stds, Stds] (Non-averaged)Filtered on Flags [Present]
    - 2 [Solvant, Meoh](Non-averaged)Filtered on Flags [Present]
    - 3 [Media, Blank] (Non-averaged)Filtered on Flags [Present]
    - 4 [Diatom-J0_ Jmax10-11](Non-averaged)Filtered on Flags [Present]
    - 3D PCA Scores Report
    - without E1-3D PCA Scores Report
    - PCA on 4113-Fold change >= 2.0
    - 5 [Diatom, J0] (Non-averaged)Filtered on Flags [Present]
    - 6 [Diatom, J1](Non-averaged)Filtered on Flags [Present]
    - 7 [Diatom, J4] (Non-averaged)Filtered on Flags [Present]
    - 8 [Diatom, J5] (Non-averaged)Filtered on Flags [Present]
      - 281 J5 Entity list of selection[8-13-14]
        - 26 Entities unic J5
      - I= J0+J1+J4_J5_J6_J8+Jmax VennDiagram Report-Article2
    - 9 [Diatom, J6] (Non-averaged)Filtered on Flags [Present]
    - 10 [Diatom, J8](Non-averaged)Filtered on Flags [Present]
    - 11 [Diatom, Jmax10-11] (Non-averaged)Filtered on Flags [Present]

- My Lists
- My Reports

Phaeodactylum tricornutum-2020

Compound	Blanc po...	Blanc po...	blanc mil...	blanc mil...	E2: Log2	E3: Log2	F1: Log2	F2: Log2	F3: Log
168.0099@6.0820003	0.199	0.351	-0.184	0.215	-0.553	-0.052	-0.439	-0.289	-0.0
168.0099@6.4369974	-0.008	0.167	-0.264	0.167	-0.520	0.008	-0.326	-0.078	0.2
168.0101@6.3350015	-0.190	0.035	-0.423	-0.095	-0.144	0.123	-0.201	-0.045	-0.0
168.0452@20.154	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.0
169.0049@1.8219997	0.395	0.246	0.847	0.688	-0.064	-0.693	-0.691	0.823	-14.0
169.0752@5.8870006	-12.756	-12.756	-12.756	-12.756	1.472	1.242	1.072	1.166	1.4
169.1501@5.431	1.727	1.023	1.940	1.210	-1.021	-16.469	-2.958	-16.469	-16.4
170.0259@6.085999	-0.005	0.081	0.051	0.089	-0.091	-0.116	0.097	-0.139	0.0
170.0563@5.8959975	1.391	1.413	0.902	1.549	-0.862	-0.154	-1.642	-0.517	-0.8
170.0926@6.7559977	4.775	1.277	-0.534	0.112	-0.340	-0.133	-0.236	-0.293	-0.7
170.0927@6.7559977	4.778	1.281	-0.529	0.105	-0.337	-0.185	-0.247	-0.290	-0.7
170.0928@6.847	4.935	1.723	-0.612	-0.378	1.261	1.516	-0.633	1.395	0.8
170.1327@20.816002	-3.889	-13.678	-13.678	-13.678	0.791	0.928	-0.184	0.755	0.6
170.1424@5.431	1.747	1.065	1.942	1.213	-1.018	-16.466	-2.956	-16.466	-16.4
171.051@1.1450003	1.016	1.276	1.116	1.176	-15.478	-0.622	-0.227	-1.398	-1.3
171.0813@20.819	-13.203	-13.203	-13.203	-13.203	1.690	1.539	-0.184	1.458	1.5
171.0899@5.316	3.132	2.491	2.974	2.449	-0.489	-1.511	-0.887	-0.961	-1.1
171.09@1.1380001	0.000	0.000	0.000	0.000	0.000	10.680	0.000	10.979	0.0
171.1472@5.455001	1.630	0.654	1.762	0.904	-0.710	-13.507	-13.507	-13.507	-13.5
171.1629@11.080997	0.792	1.205	1.114	1.558	0.029	-1.598	-0.655	0.349	-14.2
172.0893@20.820004	-15.527	-15.527	-15.527	-15.527	1.728	1.553	-0.264	1.453	1.5
173.0147@5.638	0.000	0.000	0.000	0.000	12.665	12.897	0.000	12.926	12.1
173.0335@21.368002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.0
173.034@22.722	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.0
173.0341@20.159	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.0
173.0511@8.009999	-15.172	-15.172	-15.172	-15.172	1.245	1.643	0.701	1.581	1.4
173.0692@1.1070001	-0.025	-0.175	0.118	0.085	-0.666	0.116	-0.742	-0.923	-0.8
173.1156@5.245	-13.028	-13.028	-13.028	-13.028	-13.028	-13.028	-13.028	0.225	-13.0
173.1173@5.8510003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.0
173.1281@5.7799997	0.000	0.000	0.000	0.000	14.278	14.141	0.000	14.114	13.9
174.0214@2.9920003	15.881	15.939	15.735	15.353	0.000	0.000	0.000	14.254	0.0
174.0381@2.7389991	-0.011	-0.036	-0.125	0.181	-0.540	0.099	-1.312	-0.153	0.1
174.0579@22.247992	-1.519	-1.569	-1.450	-1.587	0.204	0.195	0.011	0.100	0.7
174.0635@22.243004	-13.091	-13.091	-13.091	-13.091	1.026	1.158	0.164	0.879	1.0
174.1427@20.815	-12.973	-12.973	-12.973	-12.973	3.288	3.133	-12.973	2.979	2.9
175.0048@1.1210002	-14.232	-14.232	-14.232	-14.232	-0.555	-0.544	-0.596	-0.100	-0.7
175.0851@1.1289998	0.308	1.028	0.285	1.080	-1.149	-0.542	-0.924	-0.364	-0.6
175.1208@5.442001	14.603	15.285	14.953	15.640	0.000	0.000	0.000	0.000	0.0
175.9785@6.913	0.028	-0.078	-0.226	-12.597	0.357	-0.357	0.005	0.463	-0.0
175.9791@8.244998	-0.005	0.098	-0.255	-0.206	0.258	-0.348	0.005	0.243	0.0
175.9868@1.8100003	0.159	-0.029	0.348	0.098	0.133	-1.579	-1.955	0.592	-1.5
176.0417@9.341999	0.882	0.530	0.964	0.573	0.073	-0.423	-0.351	-0.870	-1.0
176.0477@11.403001	-14.017	-14.017	-14.017	-0.867	0.438	-0.080	0.604	1.095	-0.6
176.1204@20.817997	-12.605	-12.605	-12.605	-12.605	1.820	1.624	-0.127	1.336	1.3

Workflow

- Experiment Setup
  - Experiment Grouping
  - Create Interpretation
- Quality Control
- Analysis
- Class Prediction
  - Build Prediction Model
  - Run Prediction
- Results Interpretati...
  - Find Similar Entity L...
  - Export for Recursion
  - IDBrowser Identific...
  - Export for Identifica...
  - Export Inclusion List
  - Import Annotations

Legend - Spreadsheet (Log2 Normalized)

Rows 4113; 1 selected. Columns 35; 0 selected

414M of 509M

Recherche du phosphoenolpyruvate; Phosphoenolpyruvic acid; 138-08-9; 2-Propenoic acid, 2-(phosphonooxy)-; 2-(phosphonooxy)prop-2-enoic acid; Phosphopyruvic acid; 2-Phosphonooxyprop-2-enoic acid; PEP; ...

Compound CID: 1005 - MF: $C_3H_5O_6P$ MW: 168.04g/mol

Bizarrement ce composé est à zero partout… (en fait uniquement dans Blancs et stds…cf Profinder)

FIN